

chain nodes :

14

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

9-14

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9

exact/norm bonds :

9-14

exact bonds :

1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 14:Atom

10/810,999

=> d his

(FILE 'HOME' ENTERED AT 12:10:14 ON 18 APR 2006)

FILE 'REGISTRY' ENTERED AT 12:10:22 ON 18 APR 2006

L1 STRUCTURE UPLOADED

L2 3 S L1

L3 615 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 12:11:47 ON 18 APR 2006

L4 68 S L3

FILE 'REGISTRY' ENTERED AT 12:12:07 ON 18 APR 2006

L5 STRUCTURE UPLOADED

L6 539 S L5 SUB=L3 FUL

L7 76 S L3 NOT L6

L8 STRUCTURE UPLOADED

L9 539 S L8 SUB=L6 FUL

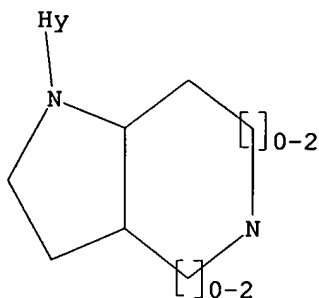
FILE 'CAPLUS' ENTERED AT 12:14:58 ON 18 APR 2006

L10 24 S L9

=> d 11

L1 HAS NO ANSWERS

L1 STR

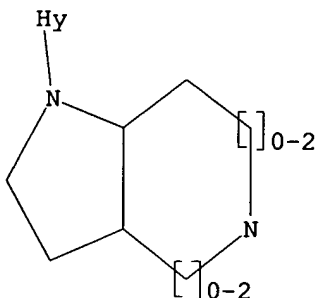


Structure attributes must be viewed using STN Express query preparation.

=> d 15

L5 HAS NO ANSWERS

L5 STR



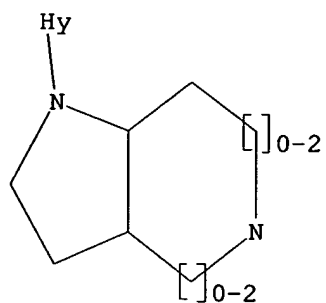
Structure attributes must be viewed using STN Express query preparation.

10/810,999

=> d 18

L8 HAS NO ANSWERS

L8 STR



Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr total

10/810,999

~~10~~ ANSWER 1 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:147715 CAPLUS

DOCUMENT NUMBER: 144:212584

TITLE: Method for the production of substituted, bicyclic
8-pyrrolidinoxanthines and their use as antidiabetic
medicaments

INVENTOR(S): Schoenafinger, Karl; Jaehne, Gerhard; Defossa,
Elisabeth; Schwink, Lothar; Wagner, Holger; Buning,
Christian; Tschank, Georg; Werner, Ulrich

PATENT ASSIGNEE(S): Sanofi-Aventis Deutschland GmbH, Germany

SOURCE: PCT Int. Appl., 40 pp.

CODEN: PIXXD2

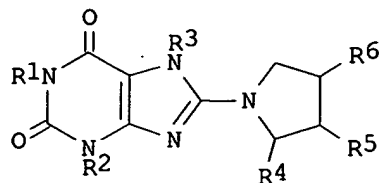
DOCUMENT TYPE: Patent

LANGUAGE: German

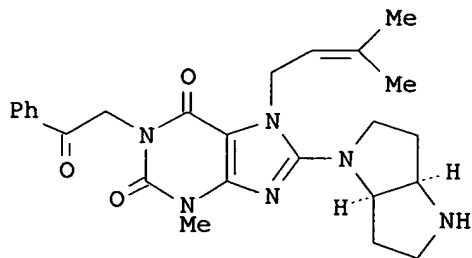
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

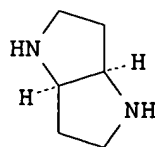
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006015701	A1	20060216	WO 2005-EP8005	20050722
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102004038270	A1	20060316	DE 2004-102004038270	20040806
PRIORITY APPLN. INFO.: GI			DE 2004-102004038270A	20040806



I



II



III

AB The invention relates to substituted, bicyclic 8-aminoxanthines, their physiol. compatible salts and to their physiol. functional derivs. The invention relates to compds. I [R1, R2, R3 = H, (un)substituted C1-6-alkyl, C3-10-cycloalkyl, C2-10-alkenyl, C2-10-alkynyl, C6-10-aryl, heterocyclyl, (optionally substituted with one or more F, Cl, Br, I, CN, NO2, SH, OH, C1-6-alkyl, CF3, OCF3, SCF3, C2-6-alkenyl, C2-6-alkynyl, OR7, OP(:O)(OR7)2, NR7R8, NR7CONR7R8, COR7, OC(:O)R7, OCO2R7, CO2R7, CONR7R8, OC(:O)NR7R8, etc.); when R4R5 = CH2CH2NH, R6 = H; when R5R6 = CH2NHCH2, R4 = H; R7, R8 = H, C1-6-alkyl, CF3, C3-10-cycloalkyl, C6-10-aryl, heterocyclyl, C1-6-alkylene-NR9R10, NR9R10, C1-6-alkylene-CO2R9, CO2R9, COR9, C1-6-alkylene-COR9, C1-6-alkylene-OR9, C1-6-alkylene-, C1-6-alkylene-S(O)NR9, SOR9, SO2R9, C1-6-alkylene-C6-10-aryl, C1-6-alkylene-heterocyclyl; R9, R10 = H, C1-6-alkyl, C1-6-alkylene-C6-10-aryl, C6-10-aryl, heterocyclyl, C1-6-alkylene-heterocyclyl; n = 0, 1, 2] and to their physiol. compatible salts. Thus, 8-pyrrolidinioxanthine II was prepared from 8-bromo-3-methyl-7-(3-methyl-3-butenyl)-1-(2-oxo-2-phenylethyl)-3,7-dihydropurin-2,6-dione (III) via reaction with cis-octahydropyrrolo[3,2-b]pyrrole. The compds. I are suited, e.g. for use as medicaments for preventing and treating type 2 diabetes (no data). The bioactivity of II was determined [IC50 = 34 nM vs. dipeptidyl peptidase IV (DPP-IV)].

IT **875877-34-2P 875877-35-3P 875877-37-5P
875877-38-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(method for the production of substituted, bicyclic 8-pyrrolidinioxanthines and their use as antidiabetic medicaments)

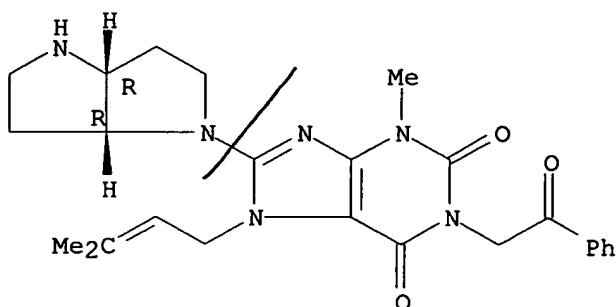
RN 875877-34-2 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,2-b]pyrrol-1(2H)-yl]-

10/810,999

3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)-,
monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

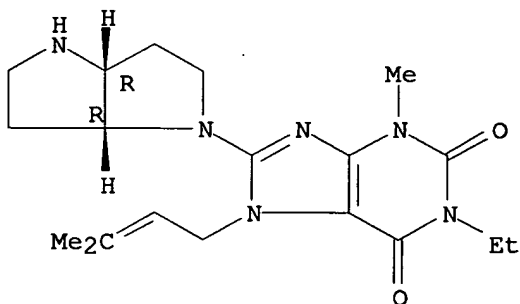


● HCl

RN 875877-35-3 CAPLUS

CN 1H-Purine-2,6-dione, 1-ethyl-8-[(3aR,6aR)-hexahydropyrrolo[3,2-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-, rel- (9CI) (CA INDEX NAME)

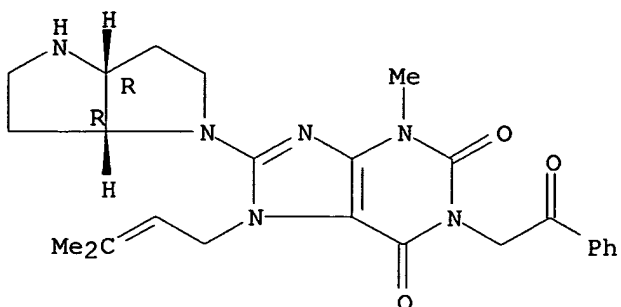
Relative stereochemistry.



RN 875877-37-5 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,2-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)- (9CI) (CA INDEX NAME)

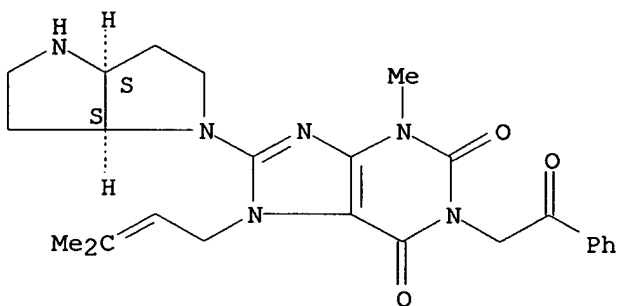
Absolute stereochemistry.



RN 875877-38-6 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,2-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/810,999

ANSWER 2 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:147681 CAPLUS

DOCUMENT NUMBER: 144:232855

TITLE: Preparation of substituted bicyclic
8-pyrrolidino-xanthines and use thereof as inhibitors
of the dipeptidyl peptidase IV

INVENTOR(S): Schoenafinger, Karl; Jaehne, Gerhard; Defossa,
Elisabeth; Schwink, Lothar; Wagner, Holger; Buning,
Christian; Tschank, Georg; Werner, Ulrich

PATENT ASSIGNEE(S): Sanofi-Aventis Deutschland GmbH, Germany

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006015699	A1	20060216	WO 2005-EP8002	20050722
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RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
DE 102004038268	A1	20060316	DE 2004-102004038268	20040806
PRIORITY APPLN. INFO.:			DE 2004-102004038268A	20040806

GI

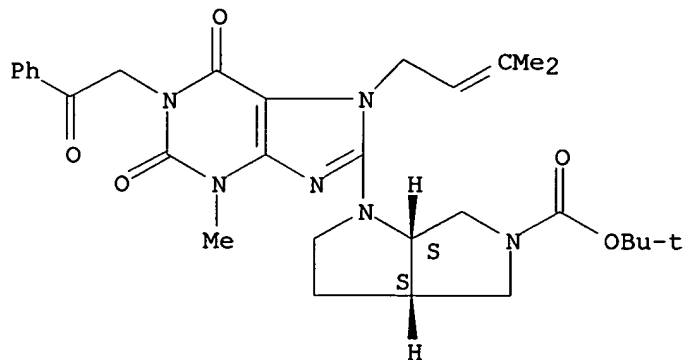
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to substituted, bicyclic 8-pyrrolidino-xanthines, to the physiol. compatible salts thereof and to the physiol. functional derivs. thereof. The invention also relates to compds. I [R1, R2, R3 = H, (un)substituted C1-10-alkyl, C3-10-cycloalkyl, C2-10-alkenyl, C2-10-alkynyl, C6-10-aryl, heterocyclyl {optionally substituted with one or more selected from F, Cl, Br, I, CN, NO2, SH, OH, C1-6-alkyl, CF3, OCF3, SCF3, C2-6-alkenyl, C2-6-alkynyl, OR7, O-P(:O)(OR7)2, NR7R8, NR7C(:O)NR7R8, C(:O)R7, O-C(:O)R7, O-CO2R7, CO2R7, CONR7R8, O-CONR7R8, (C1-6-alkylene)-OR7, (C1-6-alkylene)-NR7R8, (C1-6-alkylene)-SR7, etc.}; R4R5 = 3- to 5-membered alkylene where one CH2 = NR11 and R6 = H, R12; R5R6 = 3- to 5-membered ring where one CH2 = NR11 and R4 = H, R12; R7, R8 = H, C1-6-alkyl, CF3, C3-10-cycloalkyl, C6-10-aryl, heterocyclyl, (C1-6-alkylene)-CONR9R10, CONR9R10, (C1-6-alkylene)-CO2R9, CO2R9, COR9, (C1-6-alkylene)-COR9, (C1-6-alkylene)-OR9, (C1-6-alkylene)-NR9R10, (C1-6-alkylene)-SR9, (C1-6-alkylene)-S(O)R9, (C1-6-alkylene)-SO2R9, S(O)R9, SO2R9, (C1-4-alkylene)-aryl, (C1-4-alkylene)-heterocyclyl; R9, R10 = H, C1-6-alkyl, C6-10-aryl, (C1-6-alkylene)-(C6-10-aryl), heterocyclyl,

(C1-6-alkylene)-heterocyclyl; R11 = H, C1-6-alkyl, C3-8-cycloalkyl, (C1-4-alkylene)-aryl, (C1-4-alkylene)-heterocyclyl; R12 = F, Cl, Br, I, C1-6-alkyl, C3-8-cycloalkyl, NH₂, NH-(C1-6-alkyl), NH-(C3-7-cycloalkyl), N-(C1-6-alkyl)₂, O-(C1-6-alkyl) (alkyls may optionally be substituted with F, Cl, Br, I); n = 0 - 4], in addition to the physiol. compatible salts thereof. Thus, pyrrolopyrrole hydrochloride (\pm)-II·HCl was prepared from 8-bromo-3-methyl-7-(3-methylbut-2-enyl)-1-(2-oxo-2-phenylethyl)-3,7-dihydropurine-2,6-dione (III) via amination with cis-hexahydropyrrolo[3,4-b]pyrrole-5-carboxylic acid tert-Bu ester (IV; Boc = CO₂Me₃) in NMP containing K₂CO₃ followed by N-deprotection with HCl in EtOAc; also, the N-Boc derivative was resolved into its diastereomers and deprotected with HCl in EtOAc. The compds. can be used, for example, as medicaments for the prevention and treatment of type 2 diabetes. The inhibitory activity of II·HCl vs. dipeptidyl peptidase IV was determined [IC₅₀ = 1.6 μ M].

- IT **876130-69-7P**, 1-[3-Methyl-7-(3-methylbut-2-enyl)-2,6-dioxo-1-(2-oxo-2-phenylethyl)-2,3,6,7-tetrahydro-1H-purin-8-yl]-cis-hexahydropyrrolo[3,4-b]-5-carboxylic acid tert-butyl ester
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and N-deprotection or chromatog. resolution of; preparation of substituted bicyclic 8-pyrrolidino-xanthines and use thereof as inhibitors of the dipeptidyl peptidase IV)
- RN 876130-69-7 CAPLUS
- CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, hexahydro-1-[2,3,6,7-tetrahydro-3-methyl-7-(3-methyl-2-butenyl)-2,6-dioxo-1-(2-oxo-2-phenylethyl)-1H-purin-8-yl]-, 1,1-dimethylethyl ester, (3aR,6aR)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.



- IT **876128-02-8P 876128-03-9P 876128-06-2P**
876128-07-3P 876128-08-4P 876128-09-5P
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876128-16-4P 876128-17-5P 876128-18-6P
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876128-52-8P 876128-54-0P 876128-55-1P

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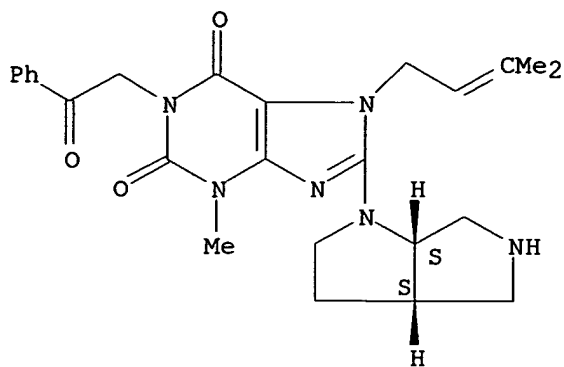
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of substituted bicyclic 8-pyrrolidino-xanthines and use thereof
 as inhibitors of the dipeptidyl peptidase IV)

RN 876128-02-8 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-
 3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)-,
 monohydrochloride, rel- (9CI) (CA INDEX NAME)

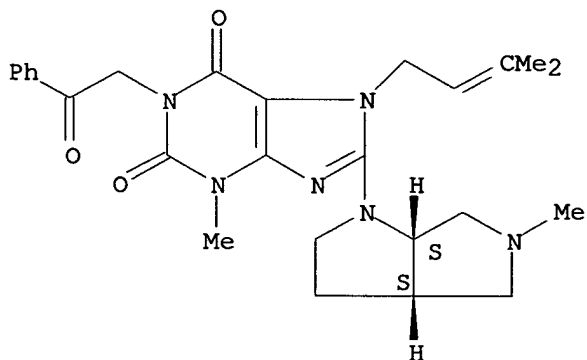
Relative stereochemistry.



● HCl

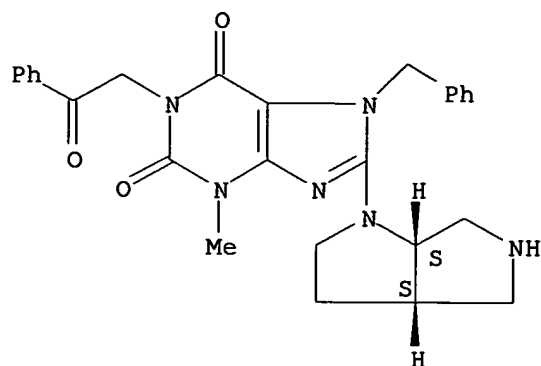
RN 876128-03-9 CAPLUS
 CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydro-5-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 876128-06-2 CAPLUS
 CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydro-5-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-phenylethyl)-7-(phenylmethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

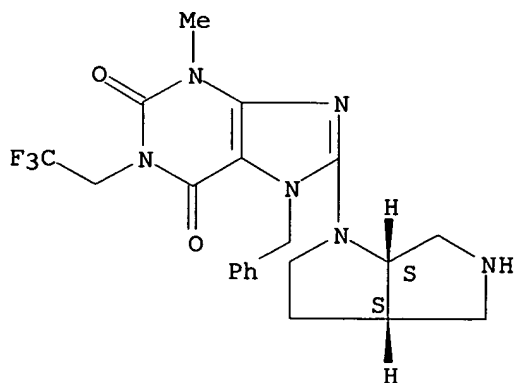
Relative stereochemistry.



● HCl

RN 876128-07-3 CAPLUS
 CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(phenylmethyl)-1-(2,2,2-trifluoroethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

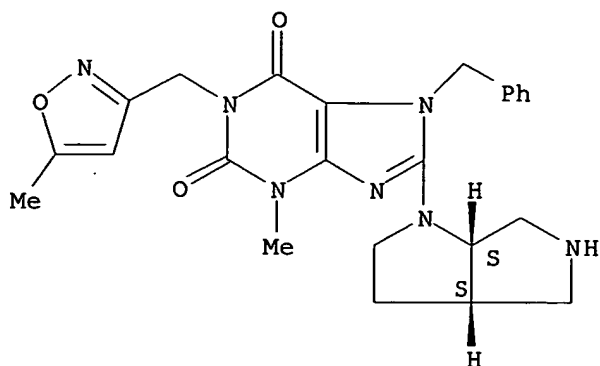
Relative stereochemistry.



● HCl

RN 876128-08-4 CAPLUS
 CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-[(5-methyl-3-isoxazolyl)methyl]-7-(phenylmethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

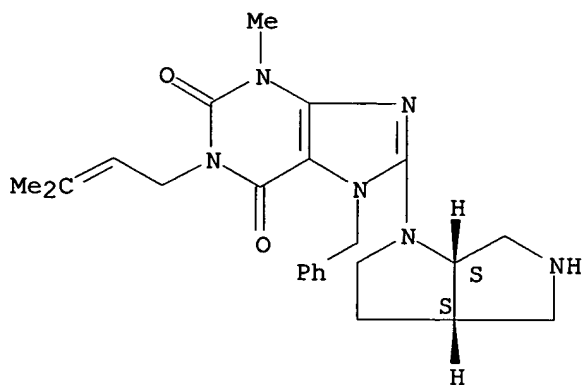


● HCl

RN 876128-09-5 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(3-methyl-2-butenyl)-7-(phenylmethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

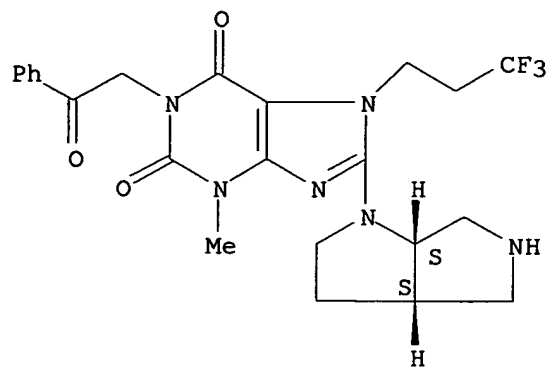


● HCl

RN 876128-10-8 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-phenylethyl)-7-(3,3,3-trifluoropropyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

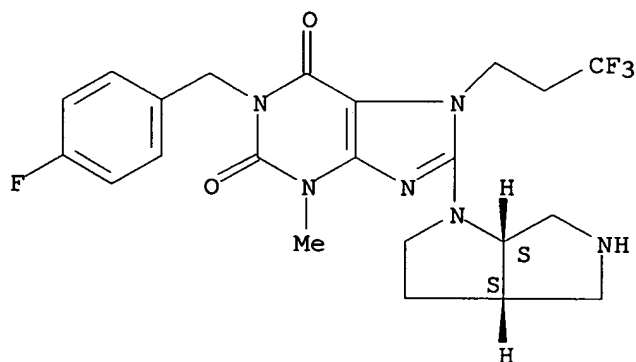


● HCl

RN 876128-11-9 CAPLUS

CN 1H-Purine-2,6-dione, 1-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3,3,3-trifluoropropyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

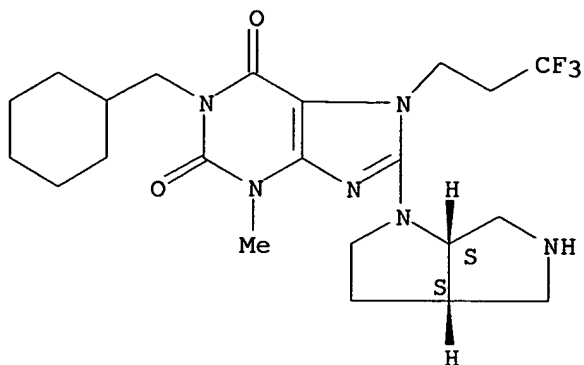


● HCl

RN 876128-12-0 CAPLUS

CN 1H-Purine-2,6-dione, 1-(cyclohexylmethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3,3,3-trifluoropropyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



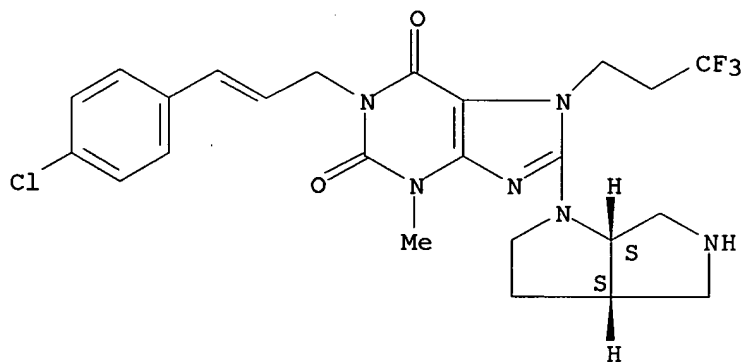
● HCl

RN 876128-13-1 CAPLUS

CN 1H-Purine-2,6-dione, 1-[3-(4-chlorophenyl)-2-propenyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3,3,3-trifluoropropyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry unknown.

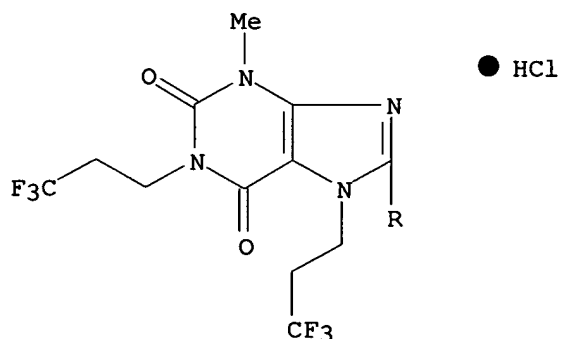
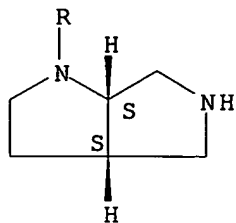


● HCl

RN 876128-14-2 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1,7-bis(3,3,3-trifluoropropyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

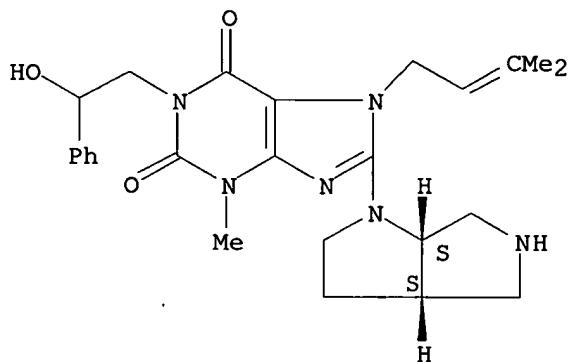
Relative stereochemistry.



RN 876128-15-3 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1-(2-hydroxy-2-phenylethyl)-3-methyl-7-(3-methyl-2-butenyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

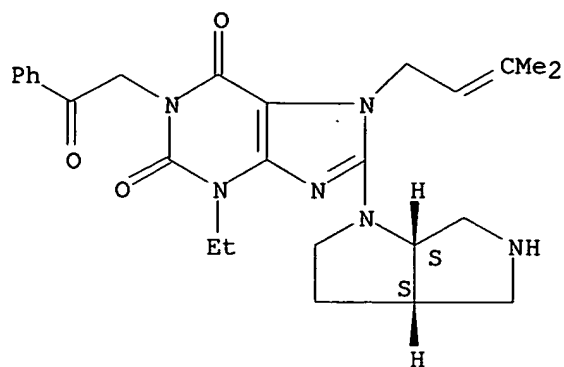


● HCl

RN 876128-16-4 CAPLUS

CN 1H-Purine-2,6-dione, 3-ethyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

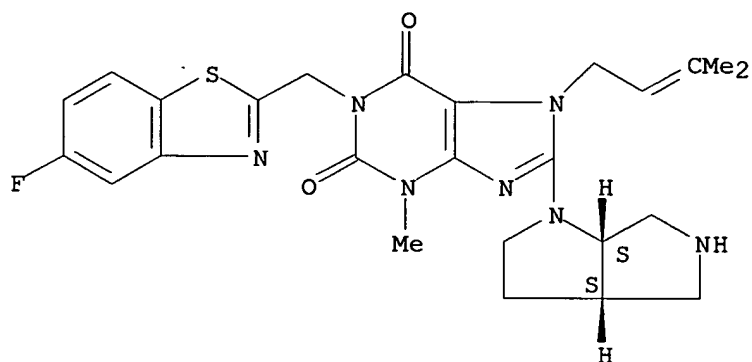


● HCl

RN 876128-17-5 CAPLUS

CN 1H-Purine-2,6-dione, 1-[(5-fluoro-2-benzothiazolyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

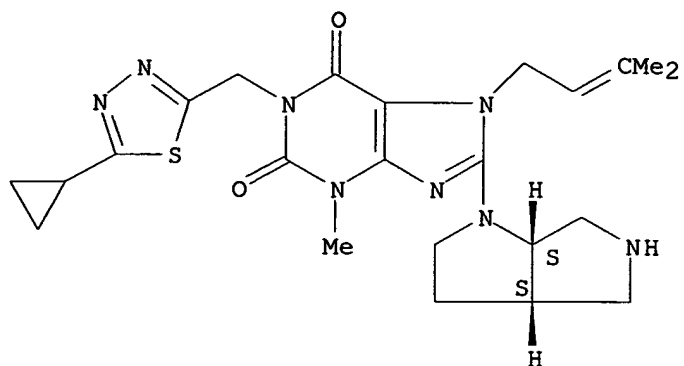


● HCl

RN 876128-18-6 CAPLUS

CN 1H-Purine-2,6-dione, 1-[(5-cyclopropyl-1,3,4-thiadiazol-2-yl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

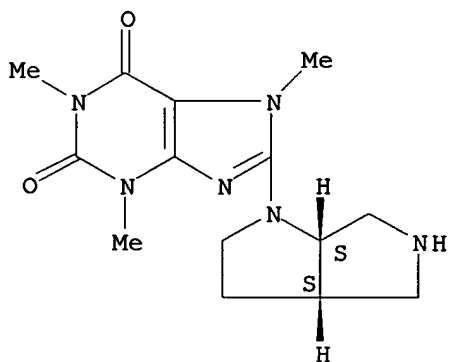


● HCl

RN 876128-19-7 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3,7-trimethyl-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

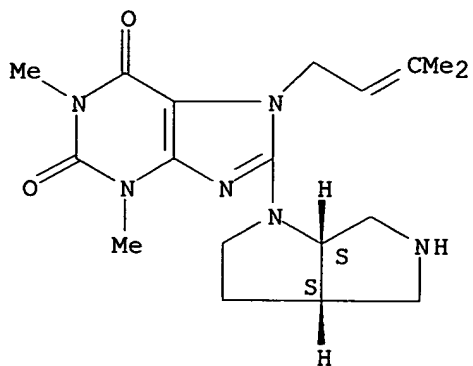


● HCl

RN 876128-20-0 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3-dimethyl-7-(3-methyl-2-butenyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

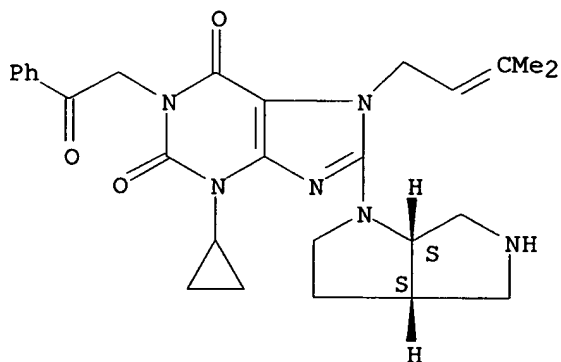


● HCl

RN 876128-21-1 CAPLUS

CN 1H-Purine-2,6-dione, 3-cyclopropyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



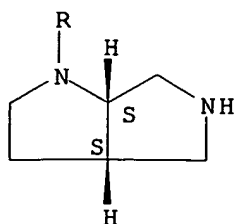
● HCl

RN 876128-22-2 CAPLUS

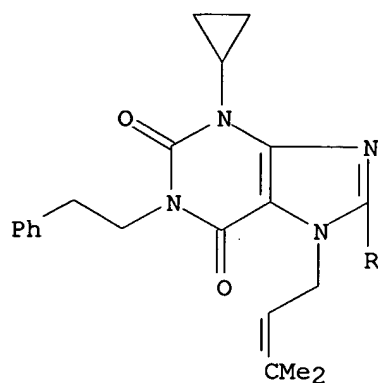
CN 1H-Purine-2,6-dione, 3-cyclopropyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-7-(3-methyl-2-butenyl)-1-(2-phenylethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

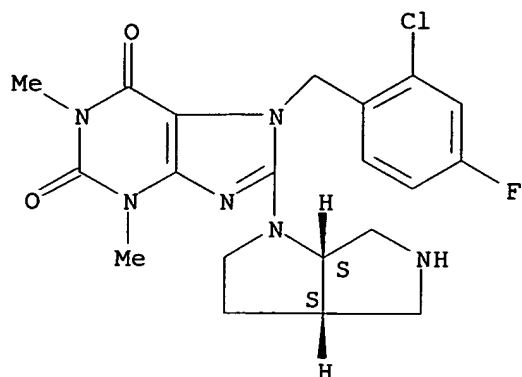


● HCl

RN 876128-23-3 CAPLUS

CN 1H-Purine-2,6-dione, 7-[(2-chloro-4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3-dimethyl-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

RN 876128-25-5 CAPLUS

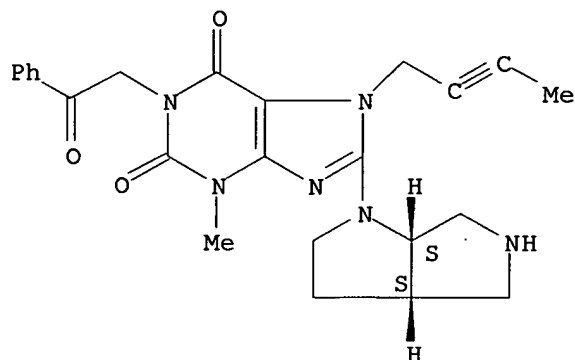
CN 1H-Purine-2,6-dione, 7-(2-butynyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-phenylethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-24-4

CMF C24 H26 N6 O3

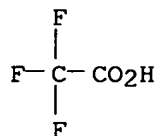
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-31-3 CAPLUS

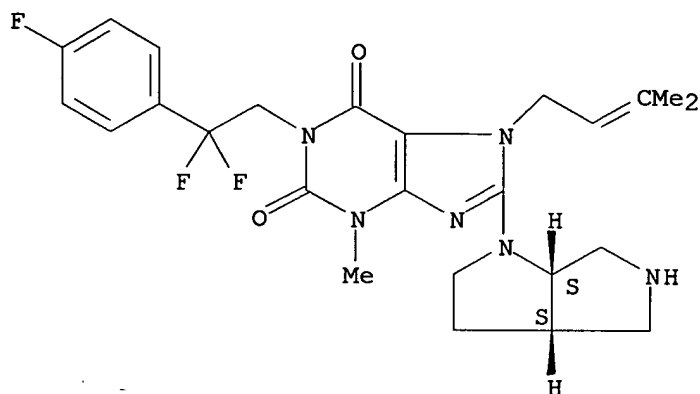
CN 1H-Purine-2,6-dione, 1-[2,2-difluoro-2-(4-fluorophenyl)ethyl]-8-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-30-2

CMF C25 H29 F3 N6 O2

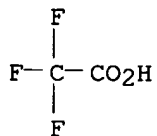
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-33-5 CAPLUS

CN 1H-Purine-2,6-dione, 1-[2,2-difluoro-2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

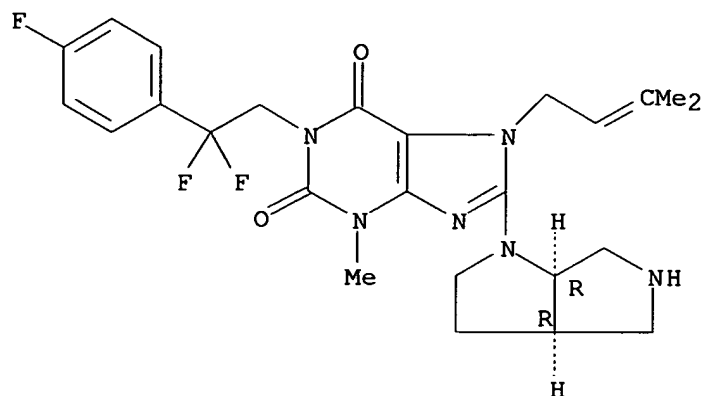
CM 1

CRN 876128-32-4

10/810,999

CMF C25 H29 F3 N6 O2

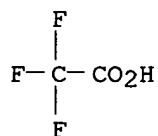
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-35-7 CAPLUS

CN 1H-Purine-2,6-dione, 3-ethyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1-(3-hydroxy-3-methylbutyl)-7-(3-methyl-2-butenyl)-, rel-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

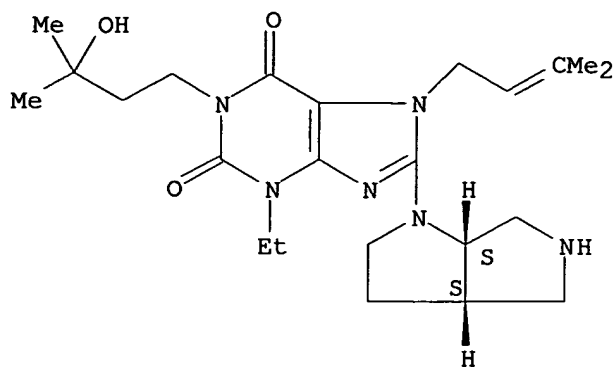
CM 1

CRN 876128-34-6

CMF C23 H36 N6 O3

Relative stereochemistry.

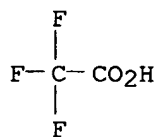
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-37-9 CAPLUS

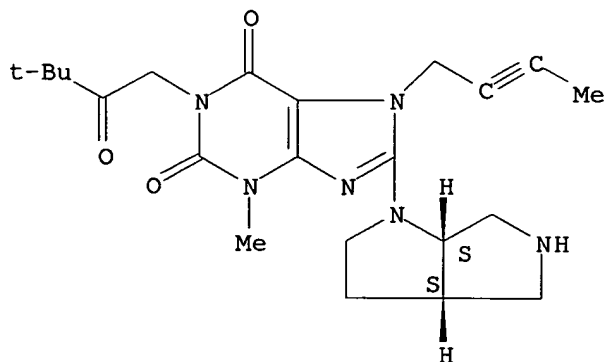
CN 1H-Purine-2,6-dione, 7-(2-butynyl)-1-(3,3-dimethyl-2-oxobutyl)-8-
[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-,
rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-36-8

CMF C22 H30 N6 O3

Relative stereochemistry.

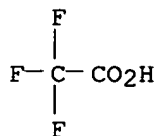


10/810,999

CM 2

CRN 76-05-1

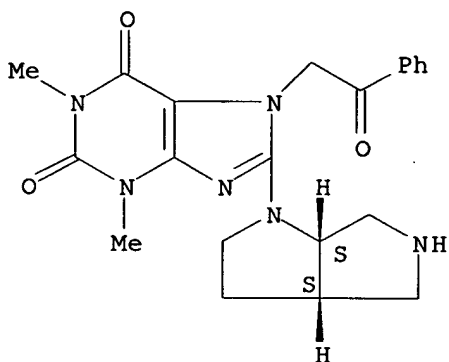
CMF C2 H F3 O2



RN 876128-38-0 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3-dimethyl-7-(2-oxo-2-phenylethyl)-, monohydrochloride, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

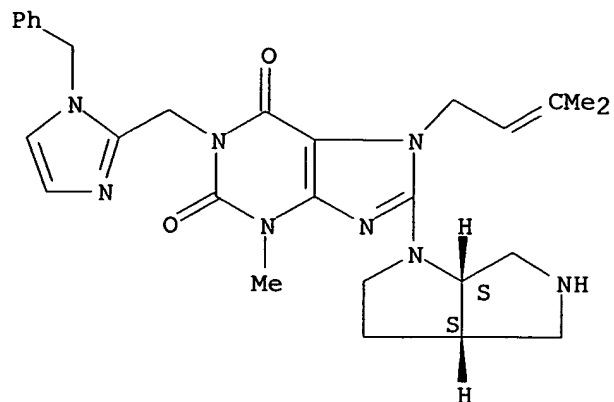


● HCl

RN 876128-39-1 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-[[1-(phenylmethyl)-1H-imidazol-2-yl]methyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 876128-41-5 CAPLUS

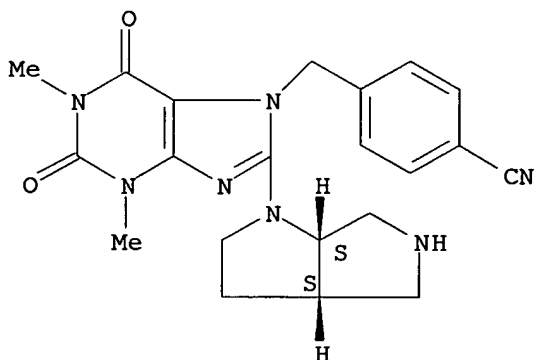
CN Benzonitrile, 4-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-7H-purin-7-yl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-40-4

CMF C21 H23 N7 O2

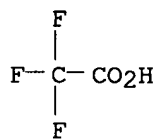
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



10/810,999

RN 876128-43-7 CAPLUS

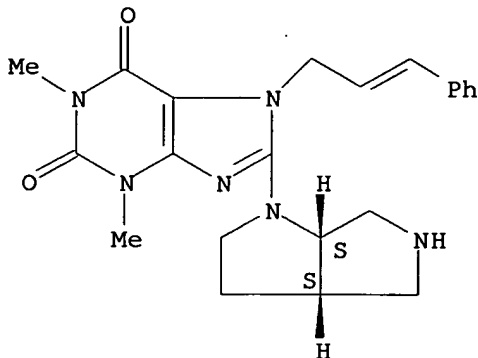
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3-dimethyl-7-(3-phenyl-2-propenyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-42-6

CMF C22 H26 N6 O2

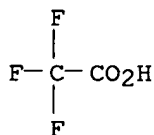
Relative stereochemistry.
Double bond geometry unknown.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-45-9 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)-3-(2,2,2-trifluoroethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

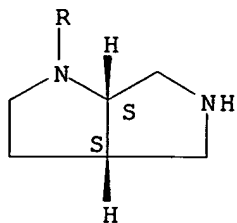
CM 1

CRN 876128-44-8

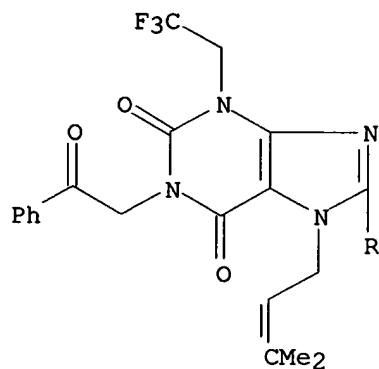
CMF C26 H29 F3 N6 O3

Relative stereochemistry.

PAGE 1-A



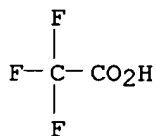
PAGE 2-A



CM 2

CRN 76-05-1

CMF C2 H F3 O2

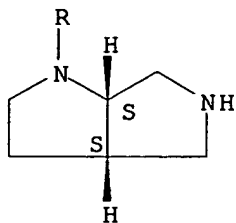


RN 876128-46-0 CAPLUS

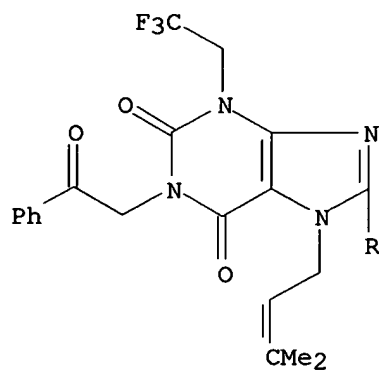
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)-3-(2,2,2-trifluoroethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



● HCl

RN 876128-48-2 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1-[(2S)-2-hydroxy-2-phenylethyl]-3-methyl-7-(3-methyl-2-butenyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

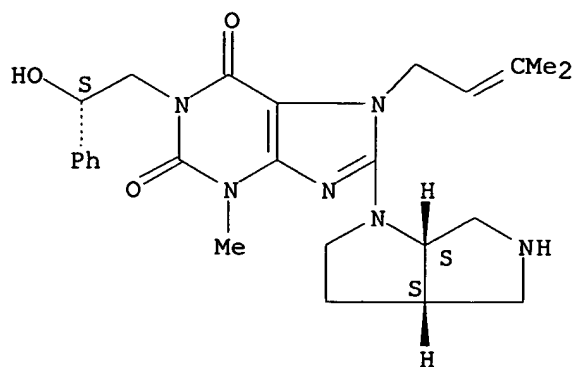
CM 1

CRN 876128-47-1

CMF C25 H32 N6 O3

Absolute stereochemistry.

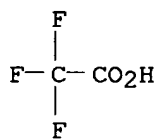
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-50-6 CAPLUS

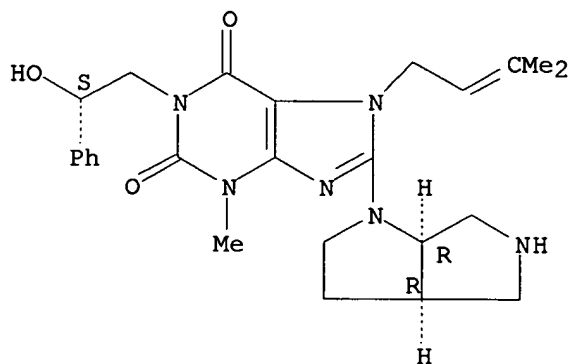
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1-[(2S)-2-hydroxy-2-phenylethyl]-3-methyl-7-(3-methyl-2-butenyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-49-3

CMF C25 H32 N6 O3

Absolute stereochemistry.

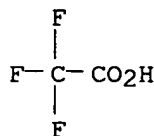


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-52-8 CAPLUS

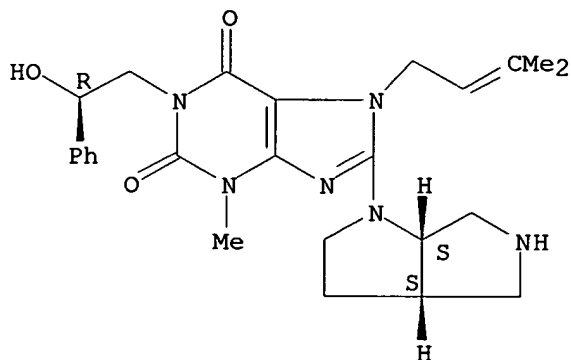
CN 1H-Purine-2,6-dione, 8-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1-[(2R)-2-hydroxy-2-phenylethyl]-3-methyl-7-(3-methyl-2-butenyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-51-7

CMF C25 H32 N6 O3

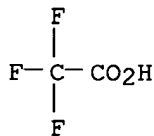
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-54-0 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1-[(2R)-2-hydroxy-2-phenylethyl]-3-methyl-7-(3-methyl-2-butenyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

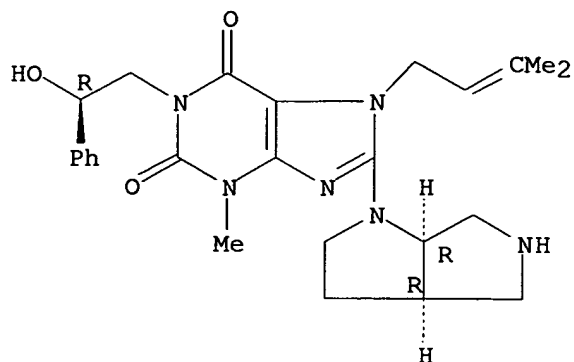
10/810,999

CM 1

CRN 876128-53-9

CMF C25 H32 N6 O3

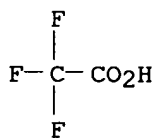
Absolute stereochemistry.



CM 2

CRN 76-05-1

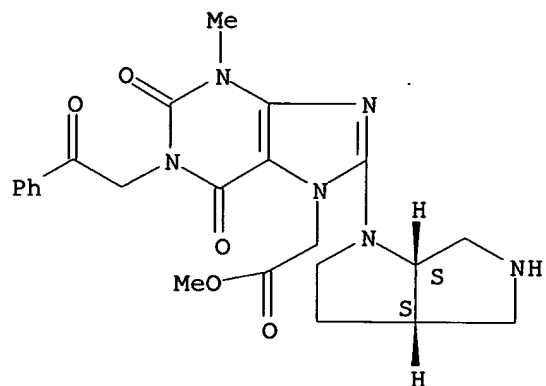
CMF C2 H F3 O2



RN 876128-55-1 CAPLUS

CN 7H-Purine-7-acetic acid, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-, methyl ester, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



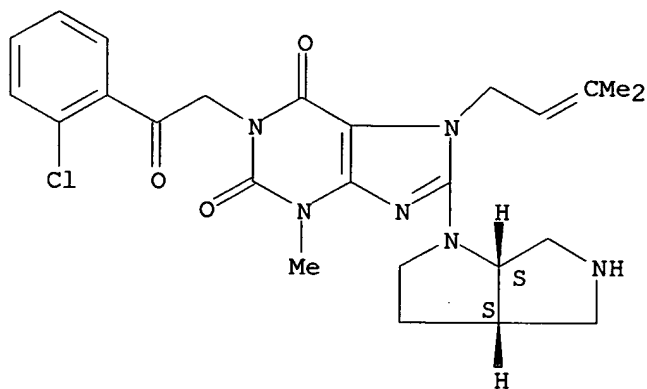
● HCl

RN 876128-57-3 CAPLUS
 CN 1H-Purine-2,6-dione, 1-[2-(2-chlorophenyl)-2-oxoethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

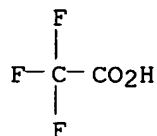
CRN 876128-56-2
 CMF C25 H29 Cl N6 O3

Relative stereochemistry.



CM 2

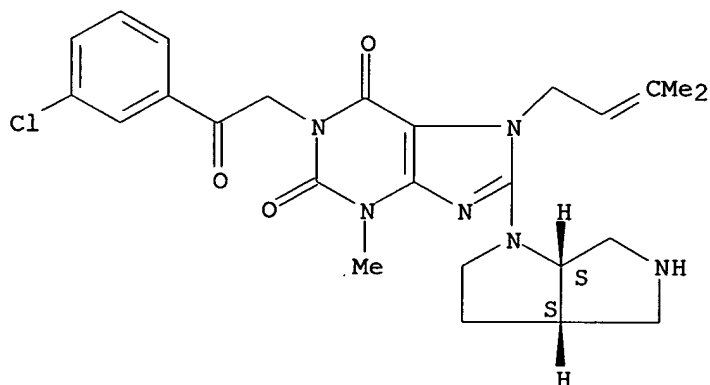
CRN 76-05-1
 CMF C2 H F3 O2



RN 876128-58-4 CAPLUS

CN 1H-Purine-2,6-dione, 1-[2-(3-chlorophenyl)-2-oxoethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-, rel- (9CI) (CA INDEX NAME)

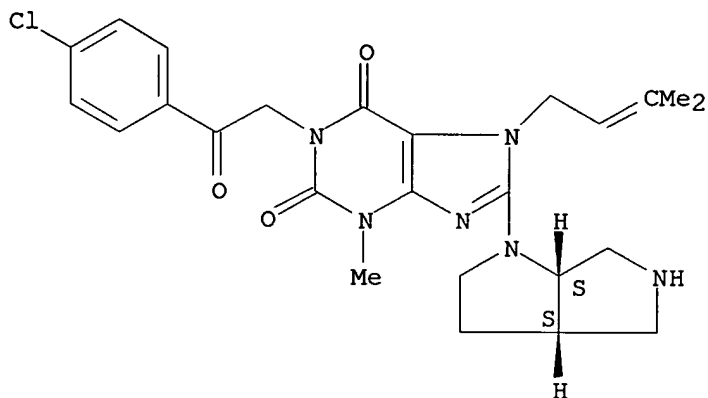
Relative stereochemistry.



RN 876128-59-5 CAPLUS

CN 1H-Purine-2,6-dione, 1-[2-(4-chlorophenyl)-2-oxoethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-, rel- (9CI) (CA INDEX NAME)

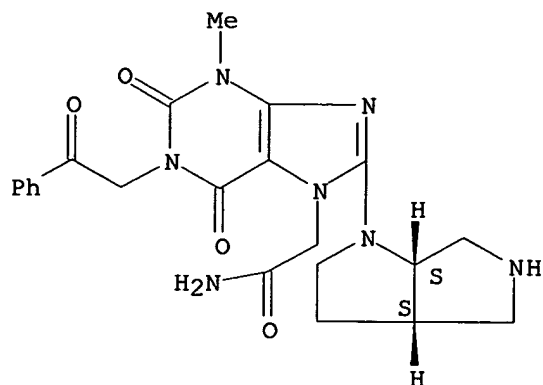
Relative stereochemistry.



RN 876128-60-8 CAPLUS

CN 7H-Purine-7-acetamide, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

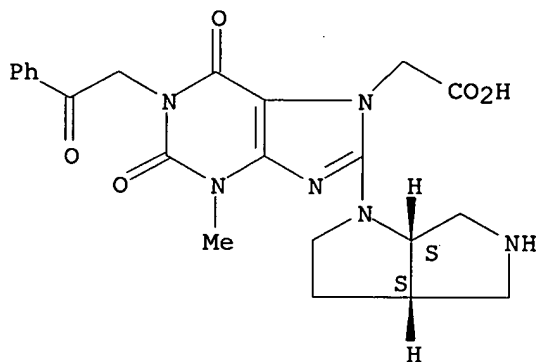


● HCl

RN 876128-61-9 CAPLUS

CN 7H-Purine-7-acetic acid, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



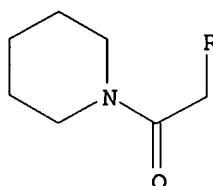
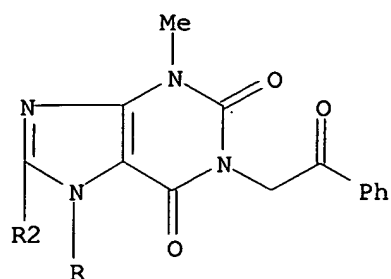
● HCl

RN 876128-62-0 CAPLUS

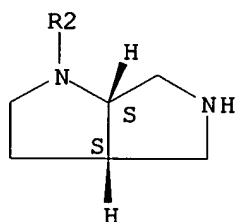
CN Piperidine, 1-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-7H-purin-7-yl]acetyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

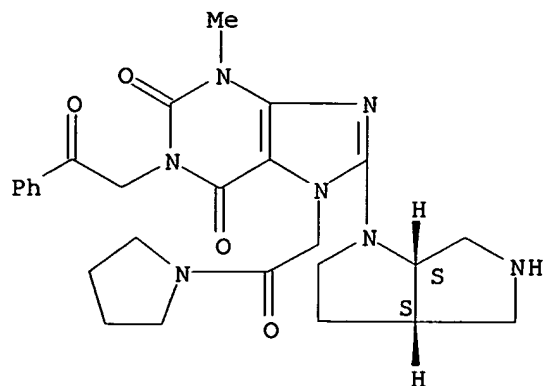


● HCl

RN 876128-63-1 CAPLUS

CN Pyrrolidine, 1-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-7H-purin-7-yl]acetyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

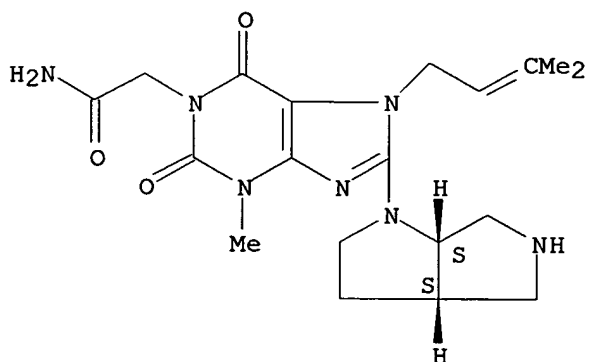


● HCl

RN 876128-64-2 CAPLUS

CN 1H-Purine-1-acetamide, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-7-(3-methyl-2-butenyl)-2,6-dioxo-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 876128-66-4 CAPLUS

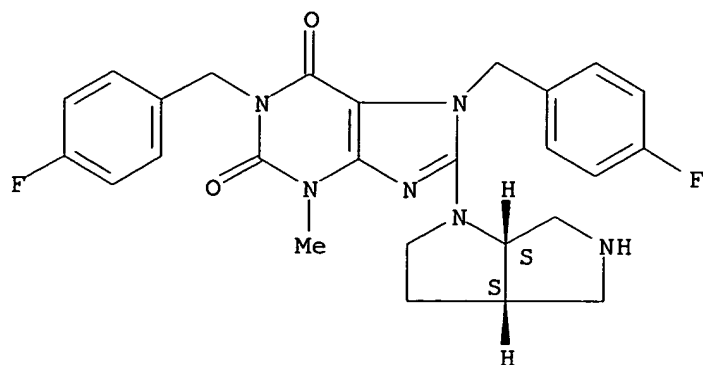
CN 1H-Purine-2,6-dione, 1,7-bis[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-65-3

CMF C26 H26 F2 N6 O2

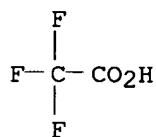
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-68-6 CAPLUS

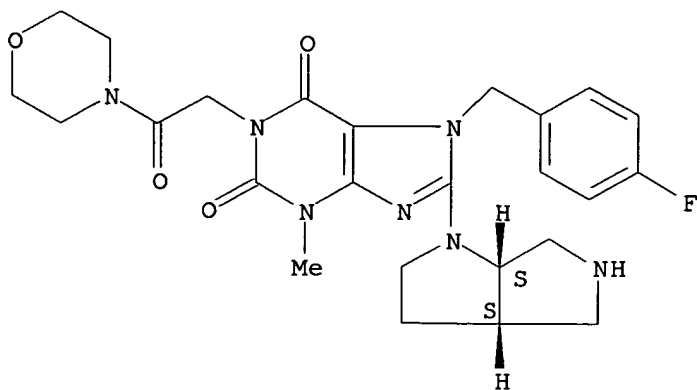
CN Morpholine, 4-[[7-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-67-5

CMF C25 H30 F N7 O4

Relative stereochemistry.

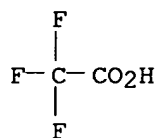


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-70-0 CAPLUS

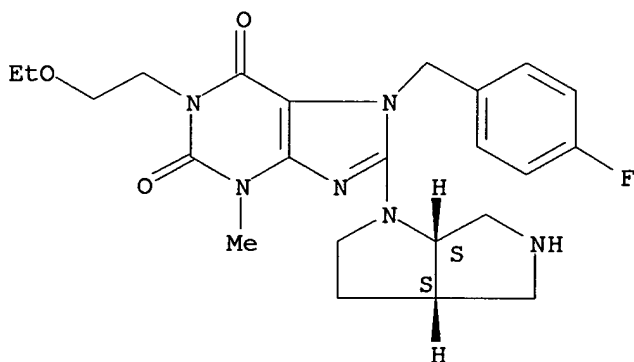
CN 1H-Purine-2,6-dione, 1-(2-ethoxyethyl)-7-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-69-7

CMF C23 H29 F N6 O3

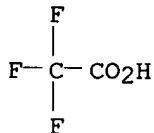
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-72-2 CAPLUS

CN 1H-Purine-2,6-dione, 7-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-

10/810,999

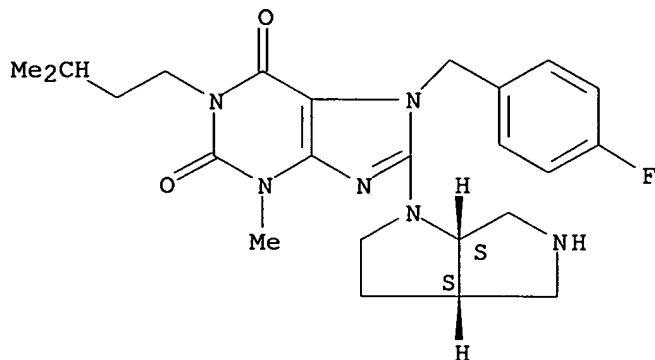
hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(3-methylbutyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-71-1

CMF C24 H31 F N6 O2

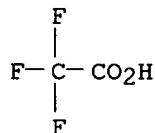
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-74-4 CAPLUS

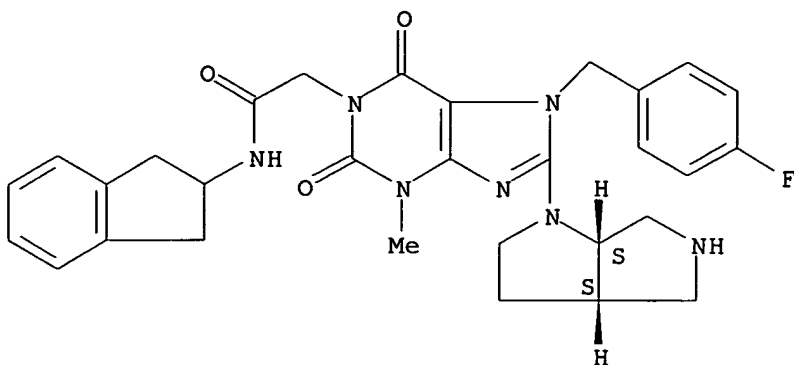
CN 1H-Purine-1-acetamide, N-(2,3-dihydro-1H-inden-2-yl)-7-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, rel, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-73-3

CMF C30 H32 F N7 O3

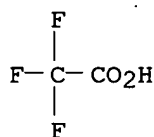
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-76-6 CAPLUS

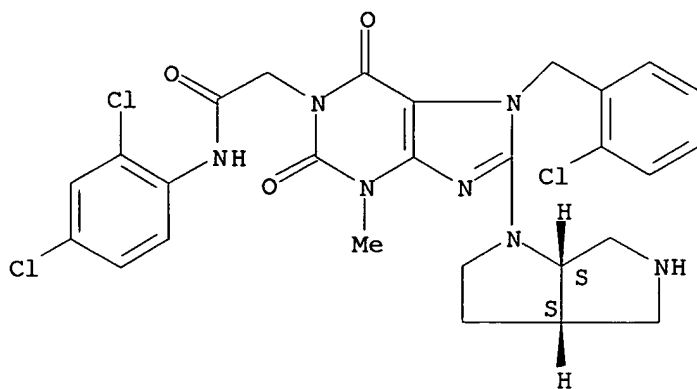
CN 1H-Purine-1-acetamide, 7-[(2-chlorophenyl)methyl]-N-(2,4-dichlorophenyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-75-5

CMF C27 H26 Cl3 N7 O3

Relative stereochemistry.

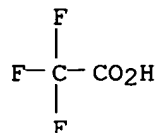


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-79-9 CAPLUS

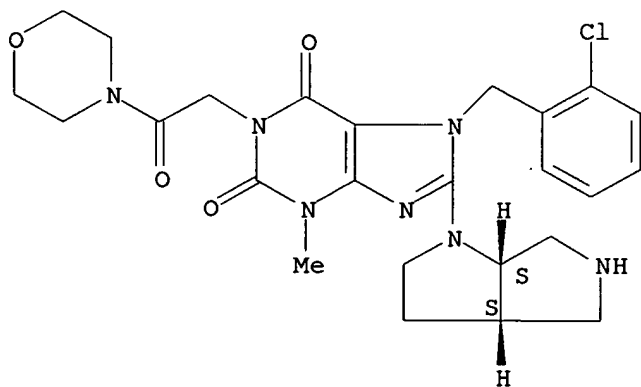
CN Morpholine, 4-[[7-[(2-chlorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-78-8

CMF C25 H30 Cl N7 O4

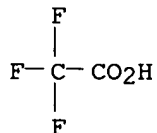
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-82-4 CAPLUS

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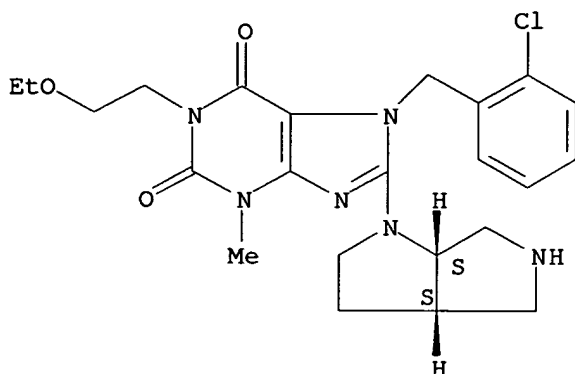
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-1-(2-ethoxyethyl)-8-
[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-,
rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-81-3

CMF C23 H29 Cl N6 O3

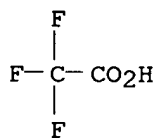
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-85-7 CAPLUS

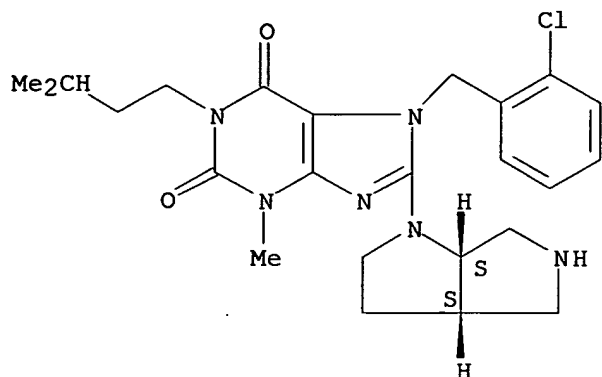
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-8-[(3aR,6aR)-
hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(3-
methylbutyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-84-6

CMF C24 H31 Cl N6 O2

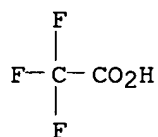
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-88-0 CAPLUS

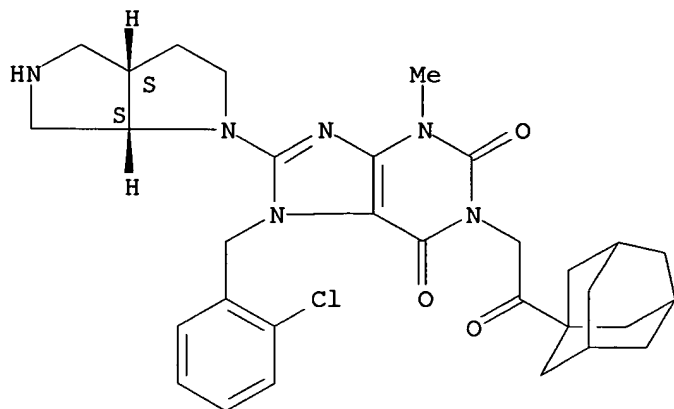
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-tricyclo[3.3.1.1^{3,7}]dec-1-ylethyl)-, rel-, mono(trifluoroacetate) (9CI)
(CA INDEX NAME)

CM 1

CRN 876128-87-9

CMF C31 H37 Cl N6 O3

Relative stereochemistry.

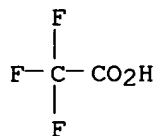


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CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-92-6 CAPLUS

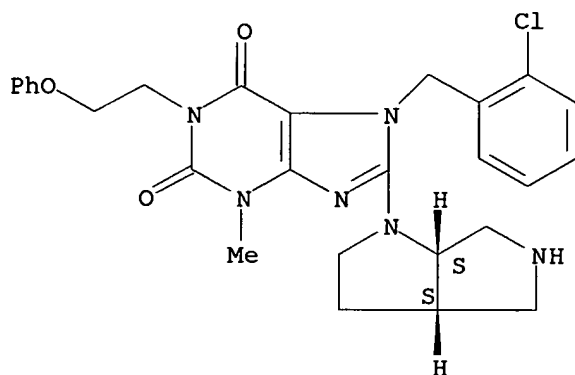
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-phenoxyethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-91-5

CMF C27 H29 Cl N6 O3

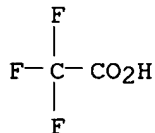
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876128-96-0 CAPLUS

CN 1H-Purine-1-acetamide, 7-[(2-chlorophenyl)methyl]-N-(2,3-dihydro-1H-inden-

10/810,999

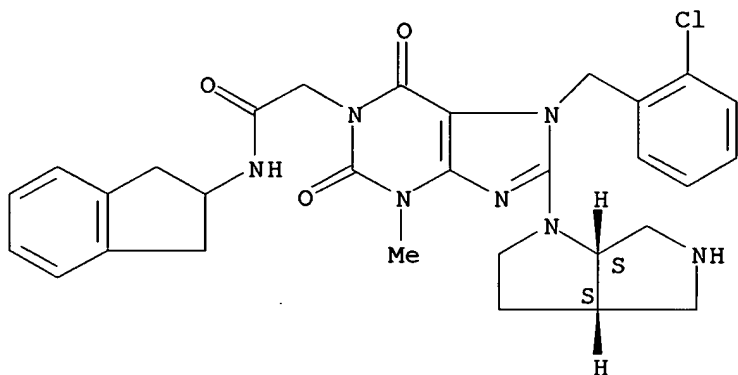
2-yl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, rel, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876128-95-9

CMF C30 H32 Cl N7 O3

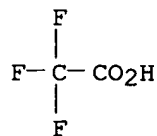
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-00-9 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3-dimethyl-7-[[3-(trifluoromethyl)phenyl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

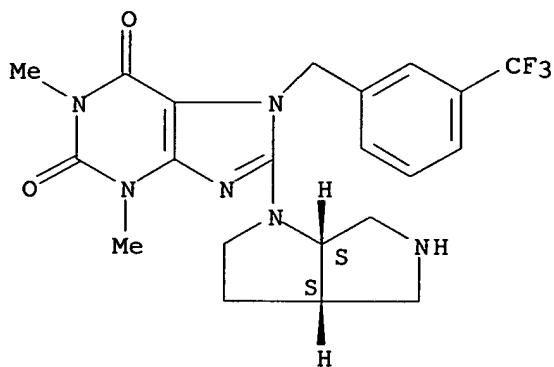
CM 1

CRN 876128-99-3

CMF C21 H23 F3 N6 O2

Relative stereochemistry.

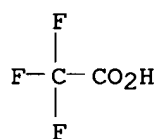
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-03-2 CAPLUS

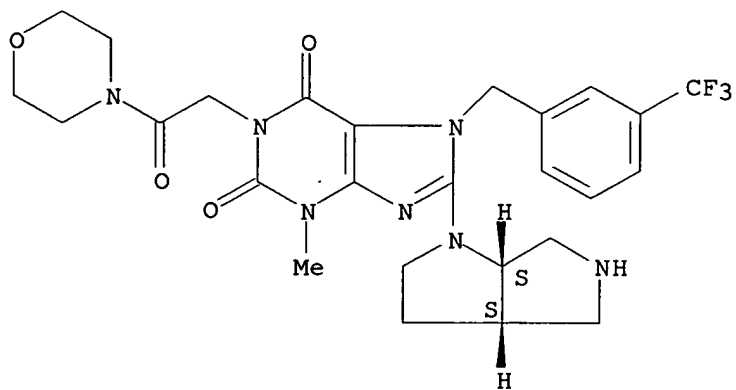
CN Morpholine, 4-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-7-[[3-(trifluoromethyl)phenyl]methyl]-1H-purin-1-yl]acetyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-02-1

CMF C26 H30 F3 N7 O4

Relative stereochemistry.

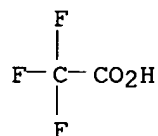


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CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-06-5 CAPLUS

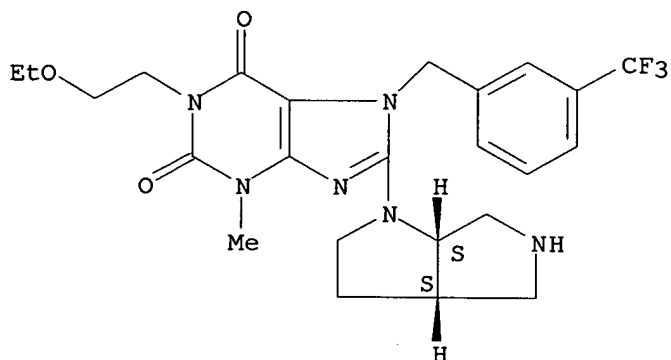
CN 1H-Purine-2,6-dione, 1-(2-ethoxyethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-[[3-(trifluoromethyl)phenyl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-05-4

CMF C24 H29 F3 N6 O3

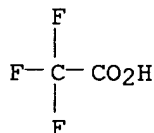
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-08-7 CAPLUS

10/810,999

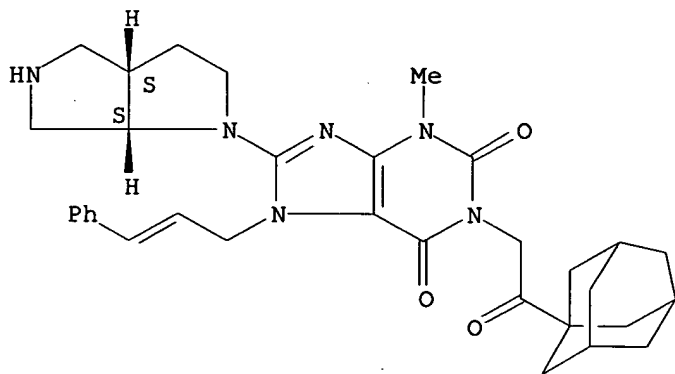
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-tricyclo[3.3.1.1^{3,7}]dec-1-ylethyl)-7-(3-phenyl-2-propenyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-07-6

CMF C33 H40 N6 O3

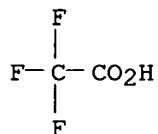
Relative stereochemistry.
Double bond geometry unknown.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-10-1 CAPLUS

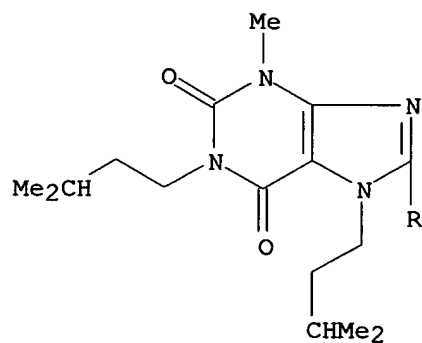
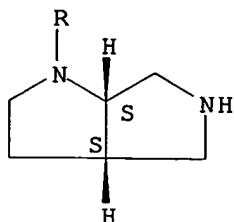
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1,7-bis(3-methylbutyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-09-8

CMF C22 H36 N6 O2

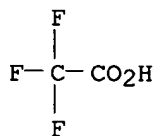
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-12-3 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methylbutyl)-1-(2-phenoxyethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

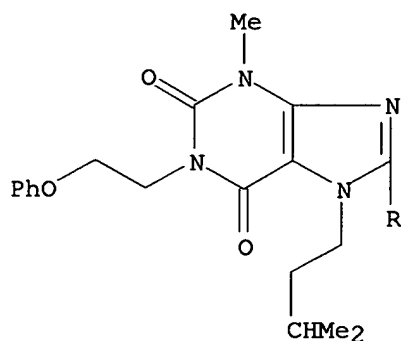
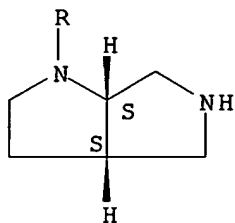
CM 1

CRN 876129-11-2

CMF C25 H34 N6 O3

Relative stereochemistry.

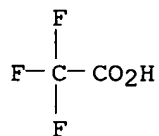
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-14-5 CAPLUS

CN 1H-Purine-2,6-dione, 1-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methylbutyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

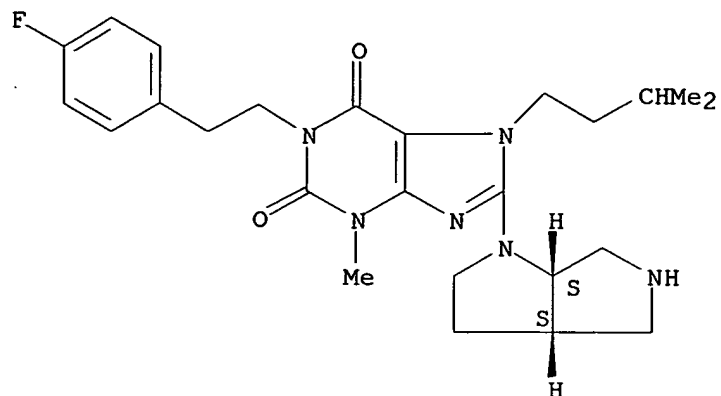
CM 1

CRN 876129-13-4

CMF C25 H33 F N6 O2

Relative stereochemistry.

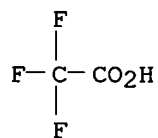
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-16-7 CAPLUS

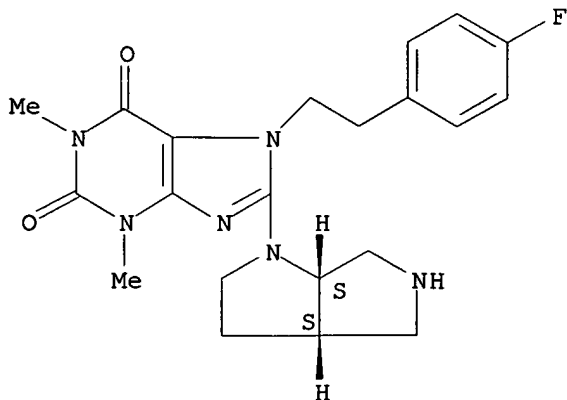
CN 1H-Purine-2,6-dione, 7-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3-dimethyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-15-6

CMF C21 H25 F N6 O2

Relative stereochemistry.

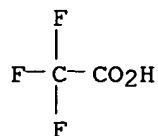


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-18-9 CAPLUS

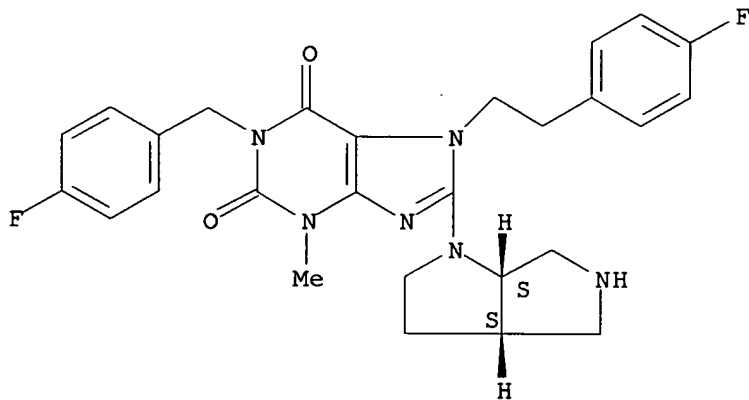
CN 1H-Purine-2,6-dione, 7-[2-(4-fluorophenyl)ethyl]-1-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-17-8

CMF C27 H28 F2 N6 O2

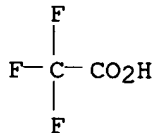
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-20-3 CAPLUS

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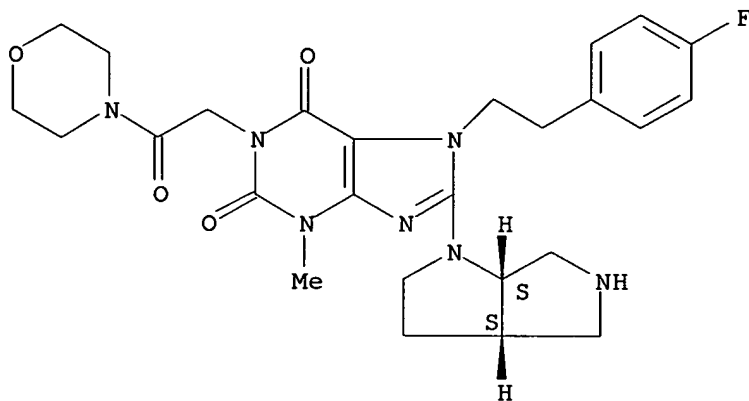
CN Morpholine, 4-[[7-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-19-0

CMF C26 H32 F N7 O4

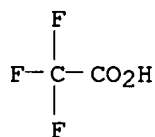
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-22-5 CAPLUS

CN 1H-Purine-2,6-dione, 1-(2-ethoxyethyl)-7-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

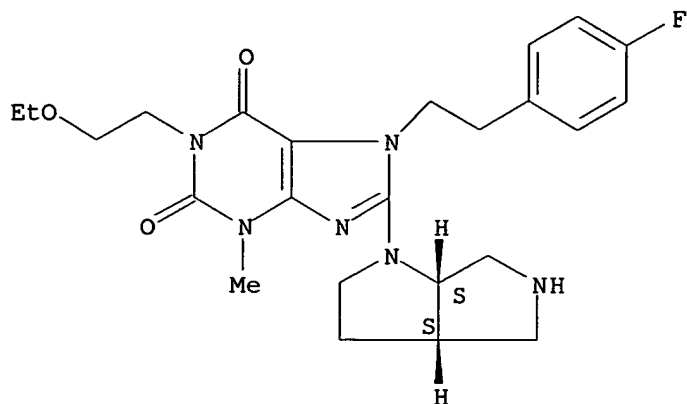
CM 1

CRN 876129-21-4

CMF C24 H31 F N6 O3

Relative stereochemistry.

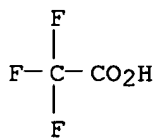
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-24-7 CAPLUS

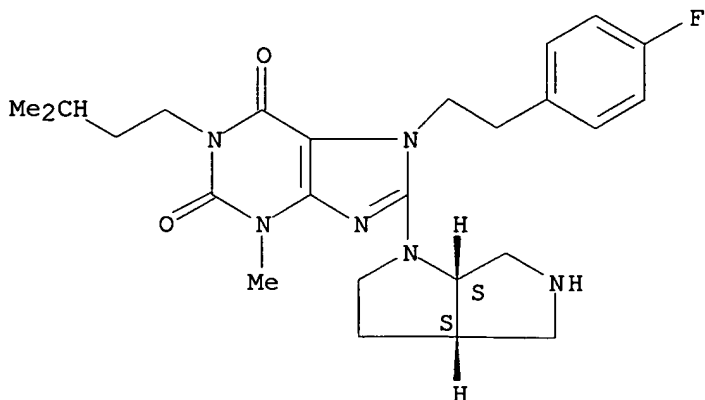
CN 1H-Purine-2,6-dione, 7-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(3-methylbutyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-23-6

CMF C25 H33 F N6 O2

Relative stereochemistry.

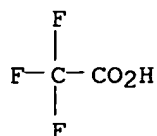


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-26-9 CAPLUS

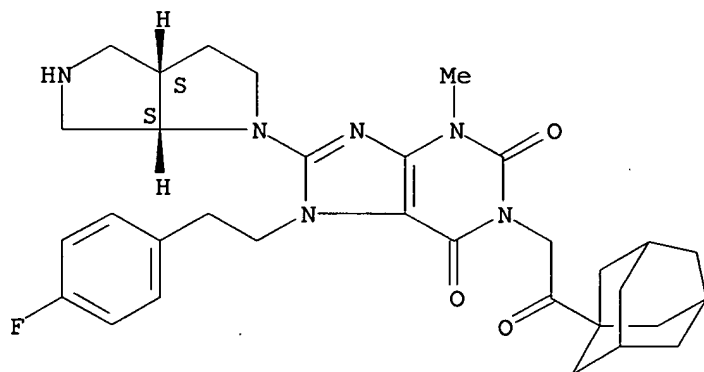
CN 1H-Purine-2,6-dione, 7-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-tricyclo[3.3.1.1^{3,7}]dec-1-ylethyl)-, rel-, mono(trifluoroacetate) (9CI)
(CA INDEX NAME)

CM 1

CRN 876129-25-8

CMF C32 H39 F N6 O3

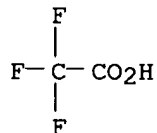
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-28-1 CAPLUS

10/810,999

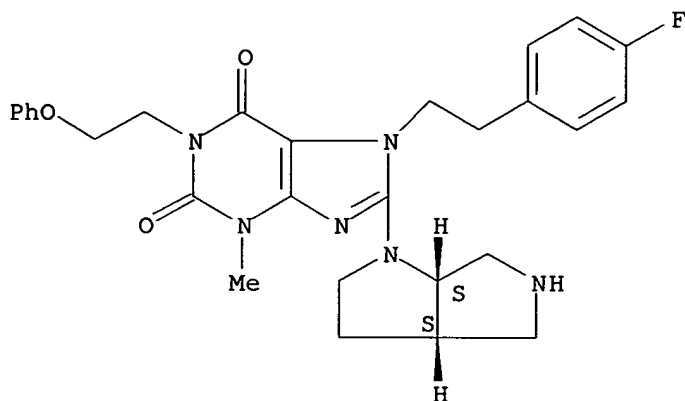
CN 1H-Purine-2,6-dione, 7-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-phenoxyethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-27-0

CMF C28 H31 F N6 O3

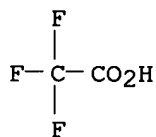
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-30-5 CAPLUS

CN 1H-Purine-1-acetamide, N-(2,3-dihydro-1H-inden-2-yl)-7-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-29-2

CMF C31 H34 F N7 O3

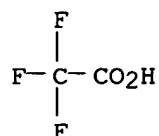
Relative stereochemistry.

10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-34-9 CAPLUS

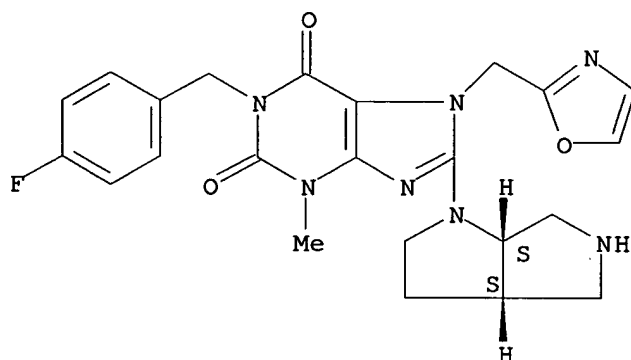
CN 1H-Purine-2,6-dione, 1-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(2-oxazolylmethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-33-8

CMF C23 H24 F N7 O3

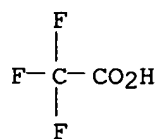
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-36-1 CAPLUS

CN 1H-Purine-1-acetamide, N-(2,4-dichlorophenyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-7-(2-

10/810,999

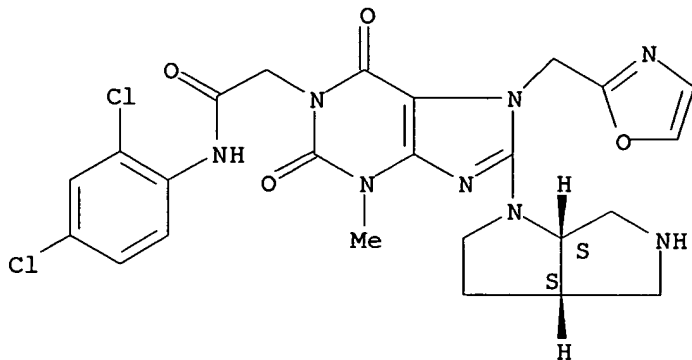
oxazolylmethyl)-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-35-0

CMF C24 H24 Cl2 N8 O4

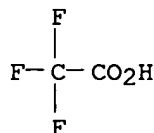
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-38-3 CAPLUS

CN 1H-Purine-2,6-dione, 1-(2-ethoxyethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(2-oxazolylmethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

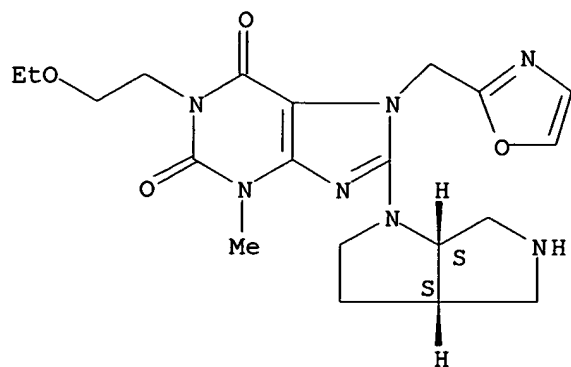
CM 1

CRN 876129-37-2

CMF C20 H27 N7 O4

Relative stereochemistry.

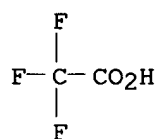
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-40-7 CAPLUS

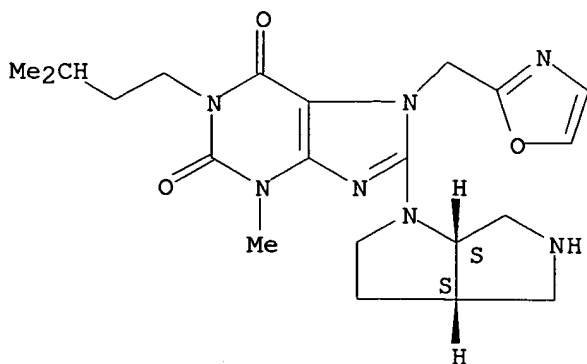
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(3-methylbutyl)-7-(2-oxazolylmethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-39-4

CMF C21 H29 N7 O3

Relative stereochemistry.

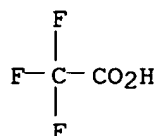


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-42-9 CAPLUS

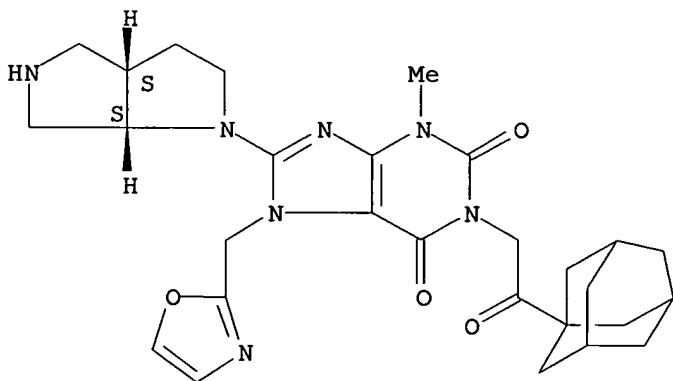
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(2-oxazolylmethyl)-1-(2-oxo-2-tricyclo[3.3.1.1^{3,7}]dec-1-ylethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-41-8

CMF C28 H35 N7 O4

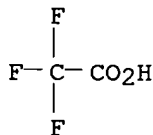
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-44-1 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-

10/810,999

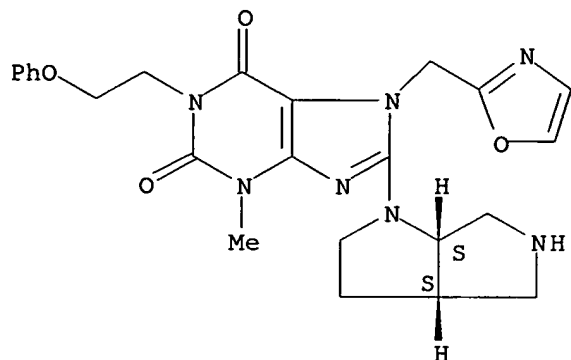
3,7-dihydro-3-methyl-7-(2-oxazolylmethyl)-1-(2-phenoxyethyl)-, rel-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-43-0

CMF C24 H27 N7 O4

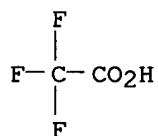
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-46-3 CAPLUS

CN 1H-Purine-2,6-dione, 1-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-
hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(2-
oxazolylmethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

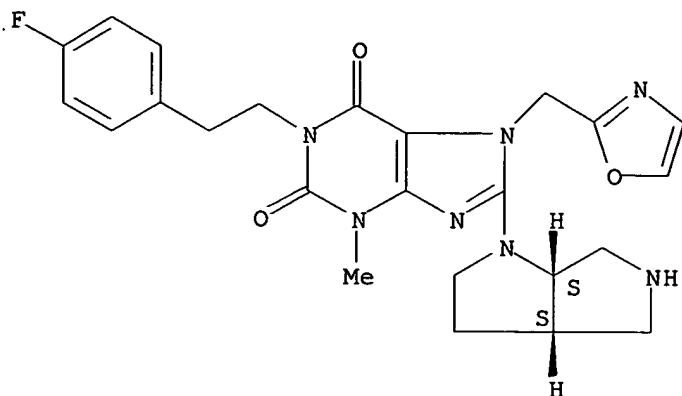
CM 1

CRN 876129-45-2

CMF C24 H26 F N7 O3

Relative stereochemistry.

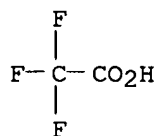
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-48-5 CAPLUS

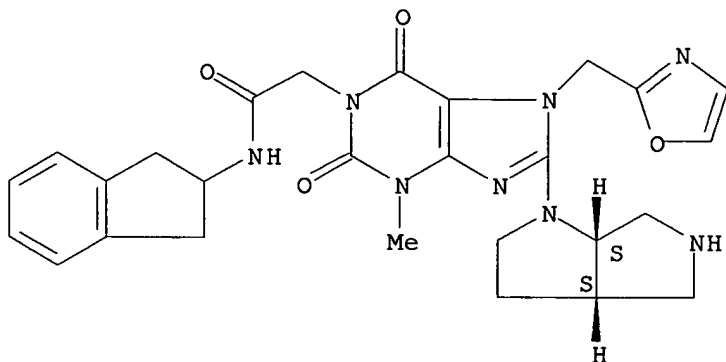
CN 1H-Purine-1-acetamide, N-(2,3-dihydro-1H-inden-2-yl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-7-(2-oxazolylmethyl)-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-47-4

CMF C27 H30 N8 O4

Relative stereochemistry.

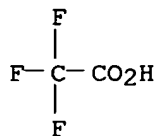


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-50-9 CAPLUS

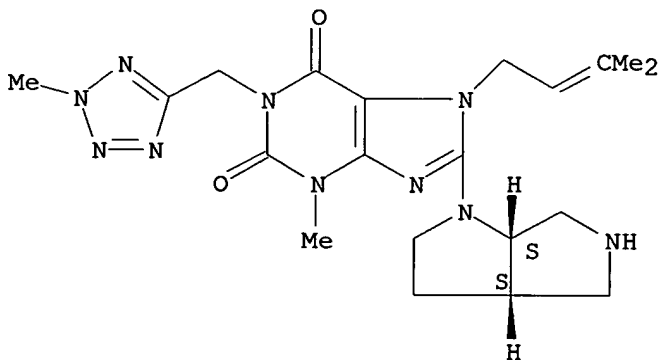
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-[(2-methyl-2H-tetrazol-5-yl)methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-49-6

CMF C20 H28 N10 O2

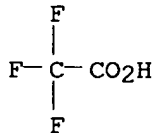
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-52-1 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-

10/810,999

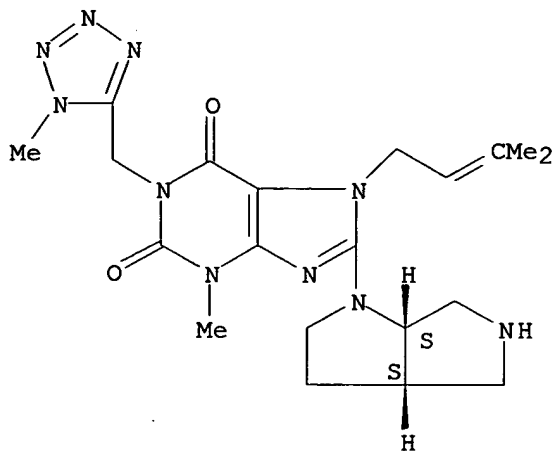
3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-[(1-methyl-1H-tetrazol-5-yl)methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-51-0

CMF C20 H28 N10 O2

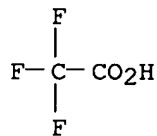
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-54-3 CAPLUS

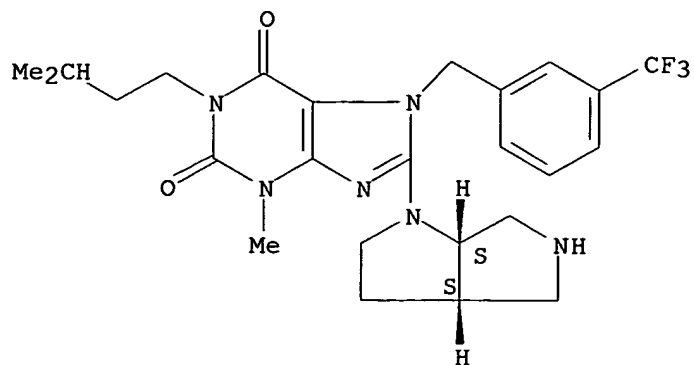
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(3-methylbutyl)-7-[[3-(trifluoromethyl)phenyl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-53-2

CMF C25 H31 F3 N6 O2

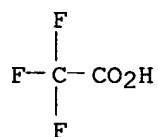
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-56-5 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-((3S,4S)-2,3,4,5-tetrahydrothiazol-5-yl)ethyl)-7-[[3-(trifluoromethyl)phenyl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

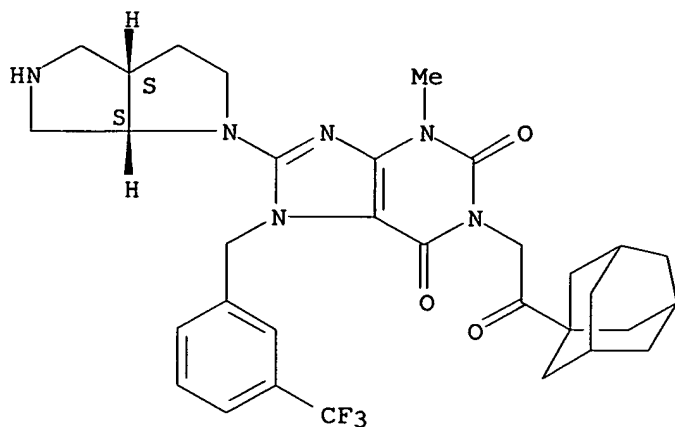
CM 1

CRN 876129-55-4

CMF C32 H37 F3 N6 O3

Relative stereochemistry.

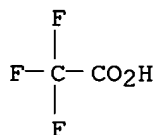
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-58-7 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-phenoxyethyl)-7-[[3-(trifluoromethyl)phenyl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

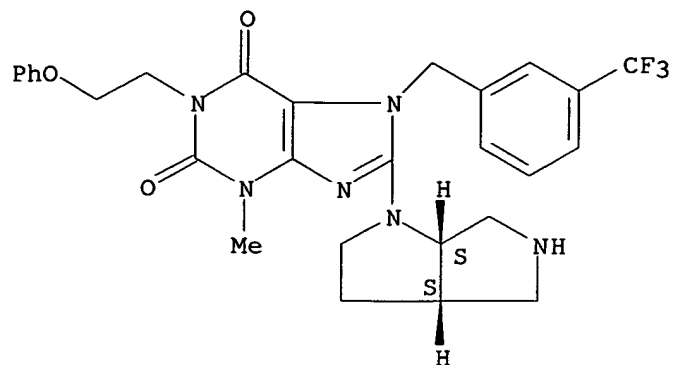
CM 1

CRN 876129-57-6

CMF C28 H29 F3 N6 O3

Relative stereochemistry.

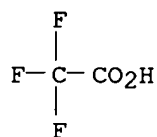
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-60-1 CAPLUS

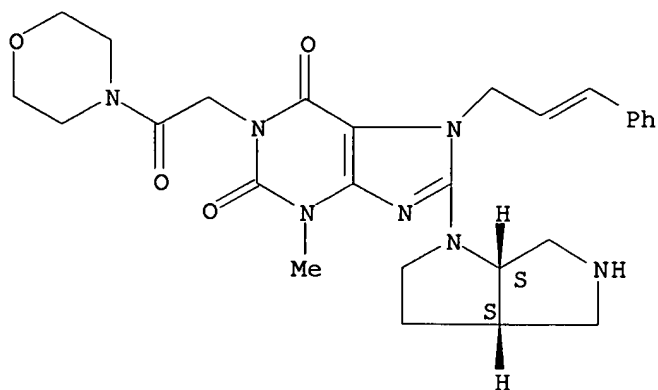
CN Morpholine, 4-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-7-(3-phenyl-2-propenyl)-1H-purin-1-yl]acetyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-59-8

CMF C27 H33 N7 O4

Relative stereochemistry.
Double bond geometry unknown.

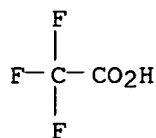


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-62-3 CAPLUS

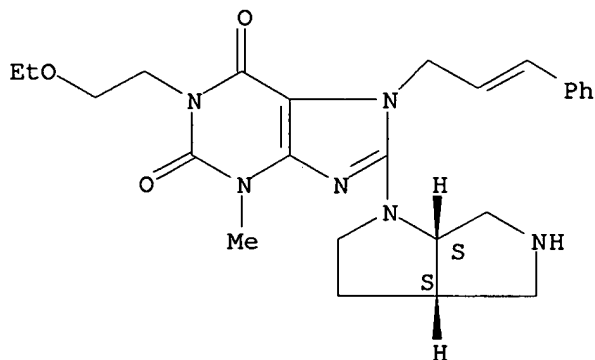
CN 1H-Purine-2,6-dione, 1-(2-ethoxyethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-phenyl-2-propenyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-61-2

CMF C25 H32 N6 O3

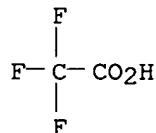
Relative stereochemistry.
Double bond geometry unknown.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-64-5 CAPLUS

10/810,999

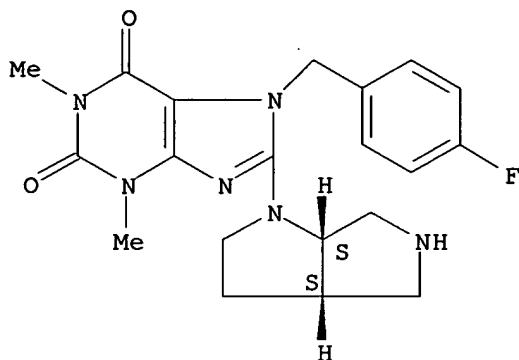
CN 1H-Purine-2,6-dione, 7-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3-dimethyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-63-4

CMF C20 H23 F N6 O2

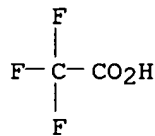
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-66-7 CAPLUS

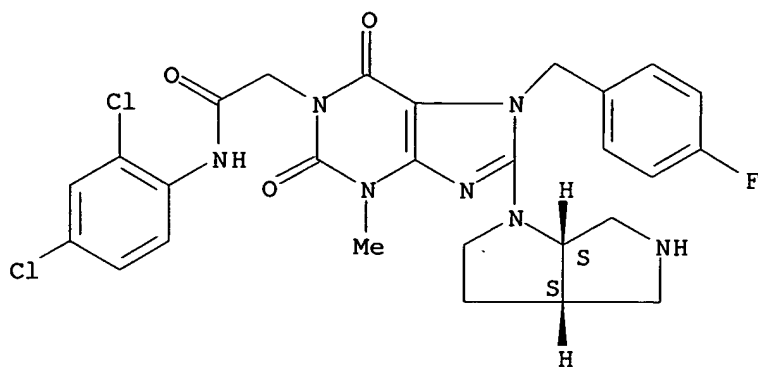
CN 1H-Purine-1-acetamide, N-(2,4-dichlorophenyl)-7-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-65-6

CMF C27 H26 Cl2 F N7 O3

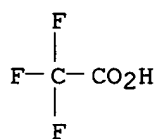
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-68-9 CAPLUS

CN 1H-Purine-2,6-dione, 7-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-tricyclo[3.3.1.1.3,7]dec-1-ylethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

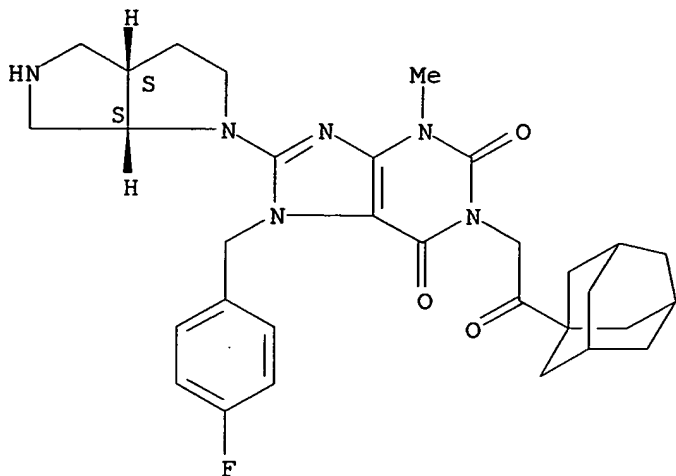
CM 1

CRN 876129-67-8

CMF C31 H37 F N6 O3

Relative stereochemistry.

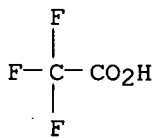
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-70-3 CAPLUS

CN 1H-Purine-2,6-dione, 1-[2-(4-fluorophenyl)ethyl]-7-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

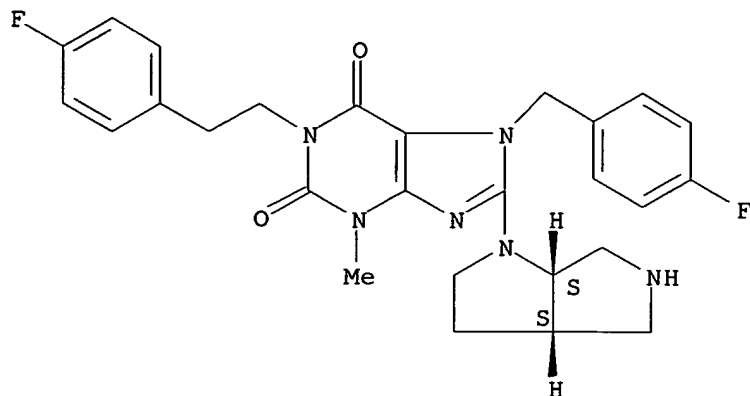
CM 1

CRN 876129-69-0

CMF C27 H28 F2 N6 O2

Relative stereochemistry.

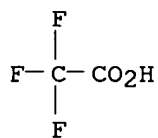
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-72-5 CAPLUS

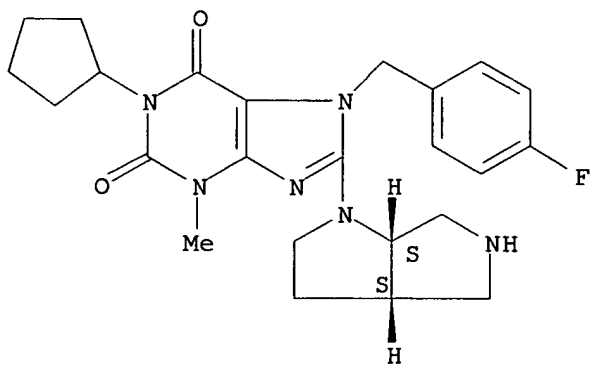
CN 1H-Purine-2,6-dione, 1-cyclopentyl-7-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-71-4

CMF C24 H29 F N6 O2

Relative stereochemistry.

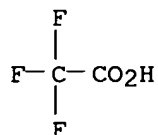


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-74-7 CAPLUS

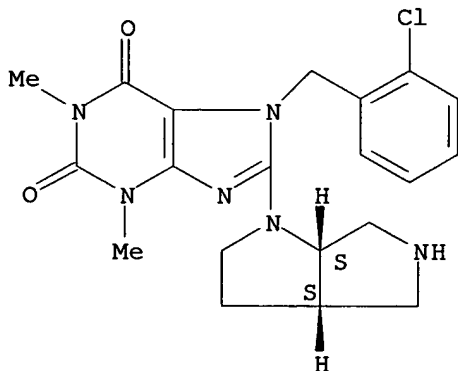
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3-dimethyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-73-6

CMF C20 H23 Cl N6 O2

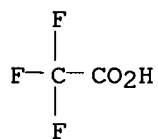
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-76-9 CAPLUS

CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-1-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-

10/810,999

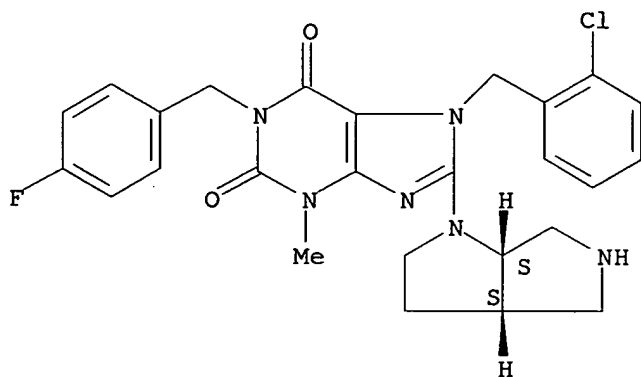
, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-75-8

CMF C26 H26 Cl F N6 O2

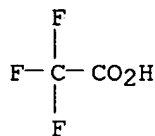
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-78-1 CAPLUS

CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-1-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

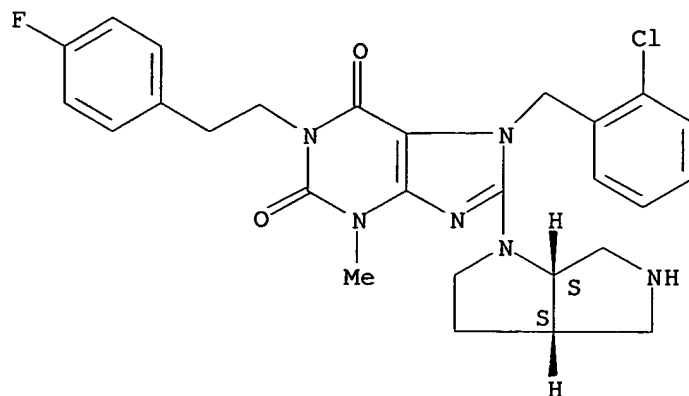
CM 1

CRN 876129-77-0

CMF C27 H28 Cl F N6 O2

Relative stereochemistry.

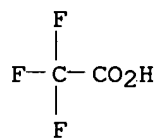
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-80-5 CAPLUS

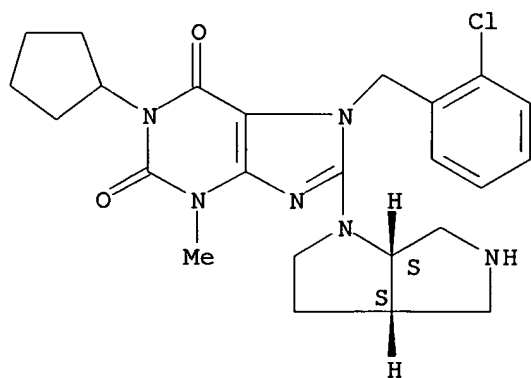
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-1-cyclopentyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-79-2

CMF C24 H29 Cl N6 O2

Relative stereochemistry.

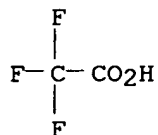


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-82-7 CAPLUS

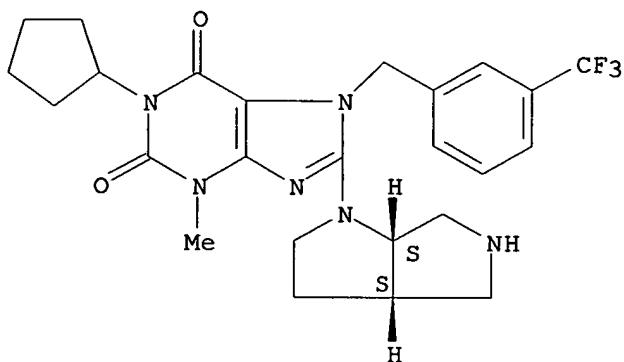
CN 1H-Purine-2,6-dione, 1-cyclopentyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-[[3-(trifluoromethyl)phenyl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-81-6

CMF C25 H29 F3 N6 O2

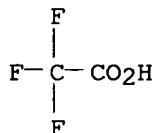
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-84-9 CAPLUS

CN 1H-Purine-1-acetamide, N-(2,3-dihydro-1H-inden-2-yl)-8-[(3aR,6aR)-

10/810,999

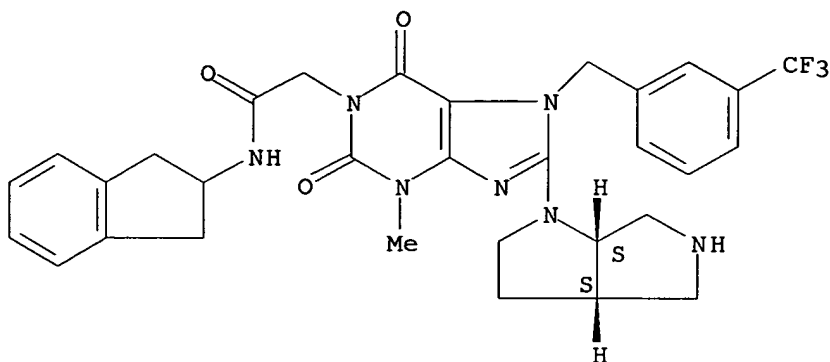
hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-7-[[3-(trifluoromethyl)phenyl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-83-8

CMF C31 H32 F3 N7 O3

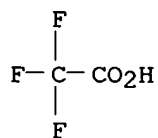
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-86-1 CAPLUS

CN 1H-Purine-2,6-dione, 7-(cyclohexylmethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1,3-dimethyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

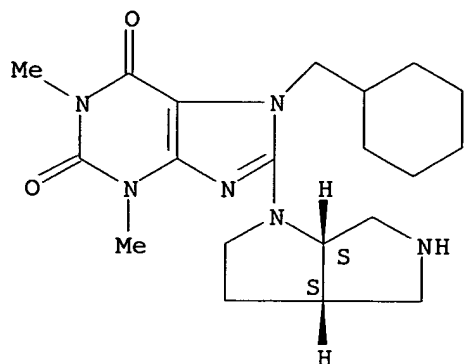
CM 1

CRN 876129-85-0

CMF C20 H30 N6 O2

Relative stereochemistry.

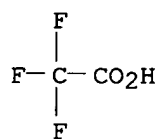
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-88-3 CAPLUS

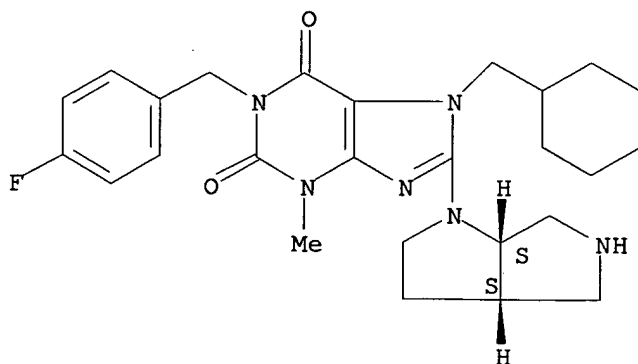
CN 1H-Purine-2,6-dione, 7-(cyclohexylmethyl)-1-[(4-fluorophenyl)methyl]-8-
[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-,
rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-87-2

CMF C26 H33 F N6 O2

Relative stereochemistry.

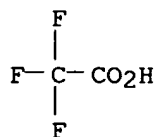


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-90-7 CAPLUS

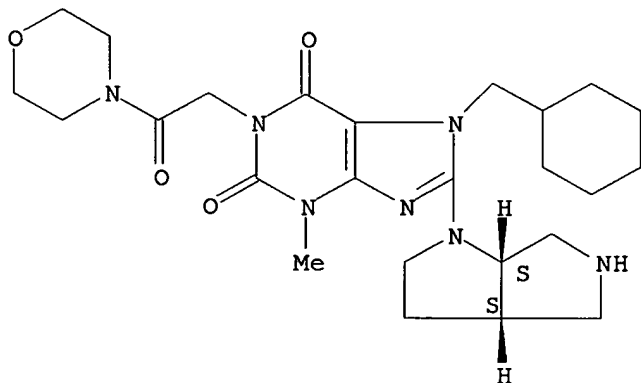
CN Morpholine, 4-[[7-(cyclohexylmethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-1-yl]acetyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-89-4

CMF C25 H37 N7 O4

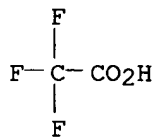
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-92-9 CAPLUS

CN 1H-Purine-2,6-dione, 7-(cyclohexylmethyl)-1-(2-ethoxyethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-,

10/810,999

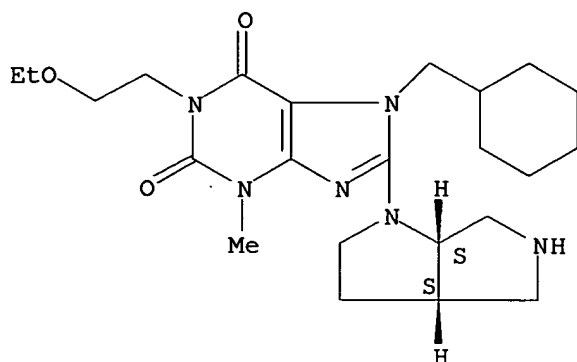
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-91-8

CMF C23 H36 N6 O3

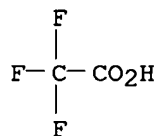
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-94-1 CAPLUS

CN 1H-Purine-2,6-dione, 7-(cyclohexylmethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(3-methylbutyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

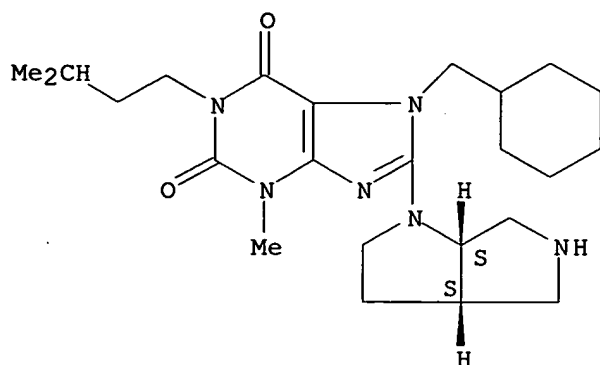
CM 1

CRN 876129-93-0

CMF C24 H38 N6 O2

Relative stereochemistry.

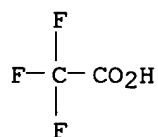
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-96-3 CAPLUS

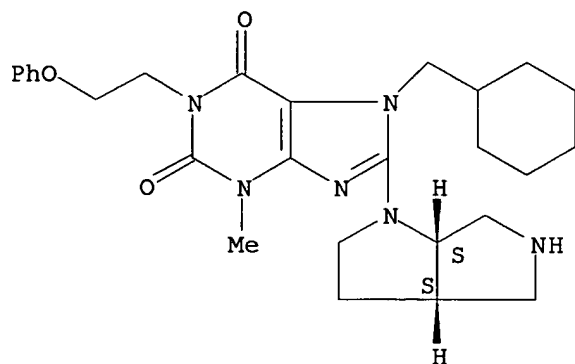
CN 1H-Purine-2,6-dione, 7-(cyclohexylmethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-phenoxyethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-95-2

CMF C27 H36 N6 O3

Relative stereochemistry.

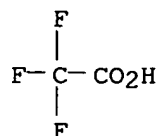


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CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876129-98-5 CAPLUS

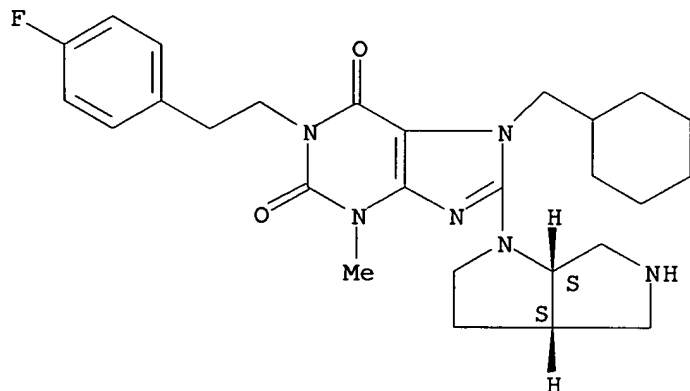
CN 1H-Purine-2,6-dione, 7-(cyclohexylmethyl)-1-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-97-4

CMF C27 H35 F N6 O2

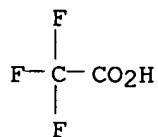
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-00-6 CAPLUS

CN 1H-Purine-1-acetamide, N-(2,3-dihydro-1H-inden-2-yl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-2,6-

10/810,999

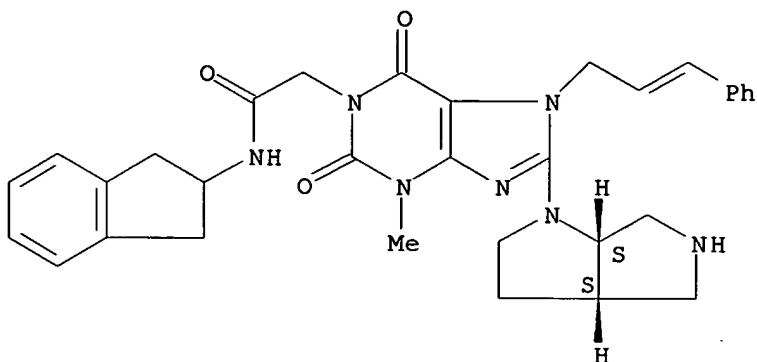
dioxo-7-(3-phenyl-2-propenyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876129-99-6

CMF C32 H35 N7 O3

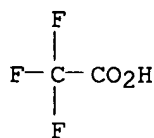
Relative stereochemistry.
Double bond geometry unknown.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-02-8 CAPLUS

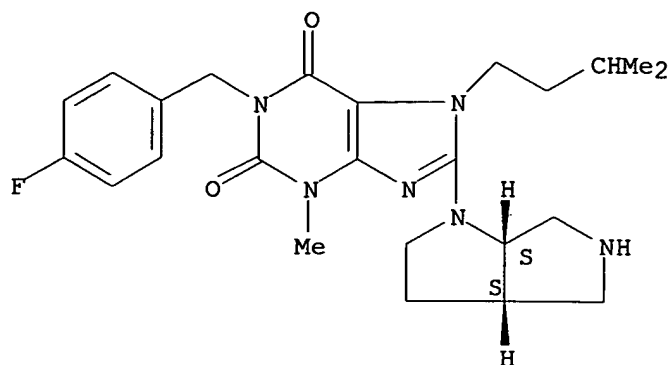
CN 1H-Purine-2,6-dione, 1-[(4-fluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methylbutyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-01-7

CMF C24 H31 F N6 O2

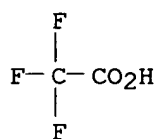
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-04-0 CAPLUS

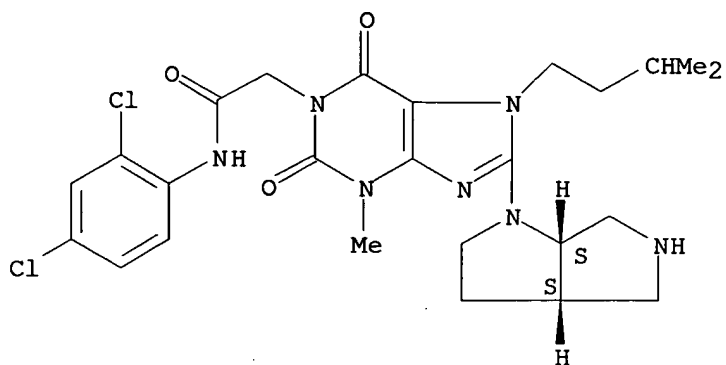
CN 1H-Purine-1-acetamide, N-(2,4-dichlorophenyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-7-(3-methylbutyl)-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-03-9

CMF C25 H31 Cl2 N7 O3

Relative stereochemistry.

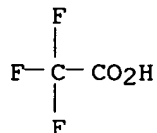


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-06-2 CAPLUS

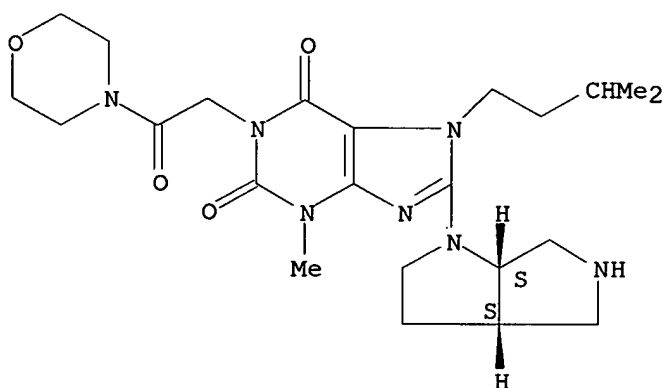
CN Morpholine, 4-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-7-(3-methylbutyl)-2,6-dioxo-1H-purin-1-yl]acetyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-05-1

CMF C23 H35 N7 O4

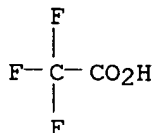
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-08-4 CAPLUS

CN 1H-Purine-2,6-dione, 1-(2-ethoxyethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-

10/810,999

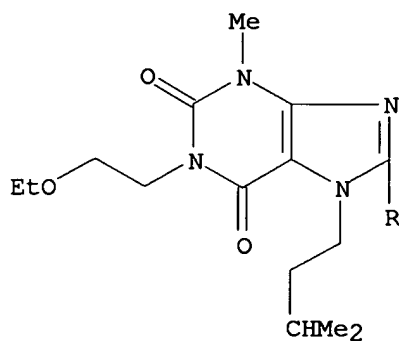
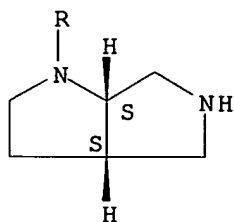
b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methylbutyl)-, rel-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-07-3

CMF C21 H34 N6 O3

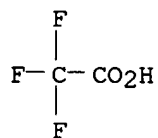
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-10-8 CAPLUS

CN 1H-Purine-2,6-dione, 1-cyclopentyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-
b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methylbutyl)-, rel-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

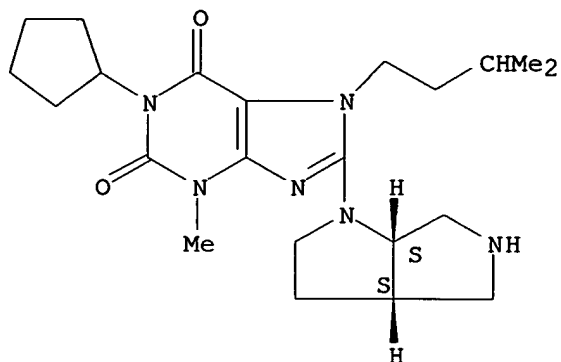
CM 1

CRN 876130-09-5

10/810,999

CMF C22 H34 N6 O2

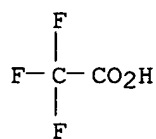
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-12-0 CAPLUS

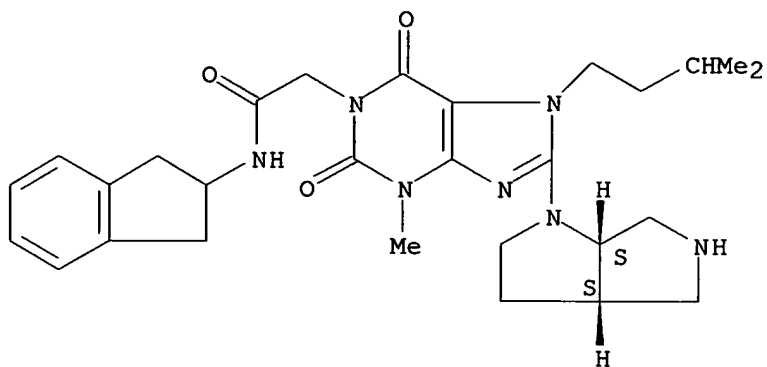
CN 1H-Purine-1-acetamide, N-(2,3-dihydro-1H-inden-2-yl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-7-(3-methylbutyl)-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-11-9

CMF C28 H37 N7 O3

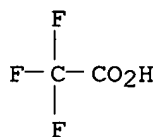
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-14-2 CAPLUS

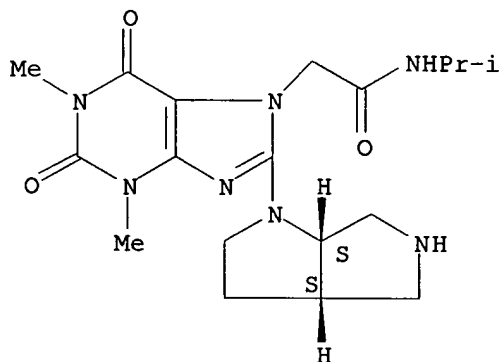
CN 7H-Purine-7-acetamide, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-1,3-dimethyl-N-(1-methylethyl)-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-13-1

CMF C18 H27 N7 O3

Relative stereochemistry.

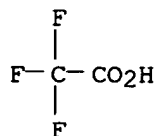


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-16-4 CAPLUS

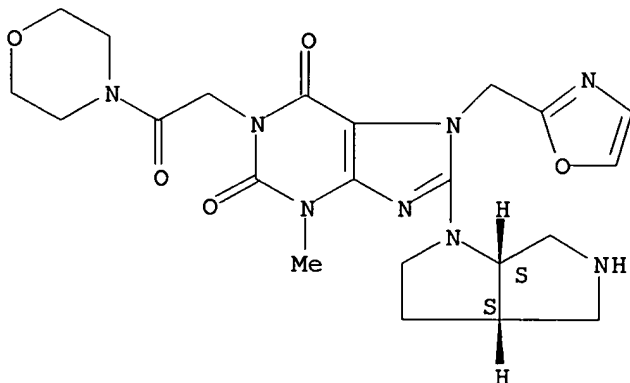
CN Morpholine, 4-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-7-(2-oxazolylmethyl)-2,6-dioxo-1H-purin-1-yl]acetyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-15-3

CMF C22 H28 N8 O5

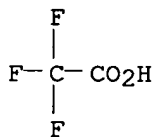
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-18-6 CAPLUS

CN 1H-Purine-2,6-dione, 1-cyclopentyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(2-oxazolylmethyl)-, rel-,

10/810,999

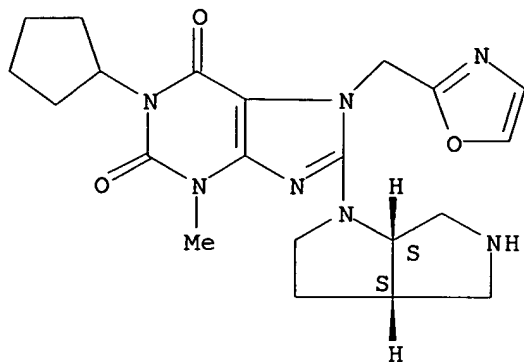
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-17-5

CMF C21 H27 N7 O3

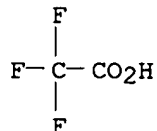
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-20-0 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-[(2-methyl-2H-tetrazol-5-yl)methyl]-1-(2-oxo-2-phenylethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

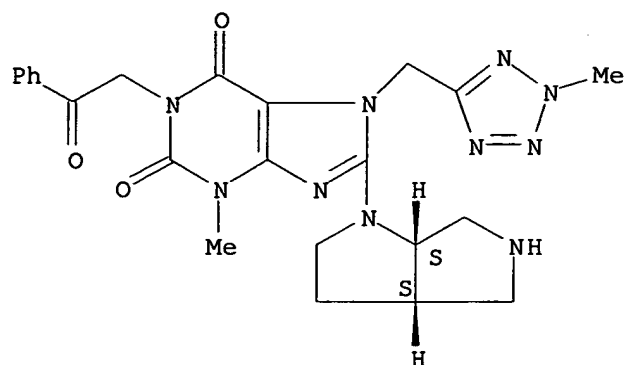
CM 1

CRN 876130-19-7

CMF C23 H26 N10 O3

Relative stereochemistry.

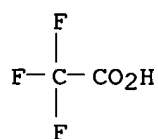
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-22-2 CAPLUS

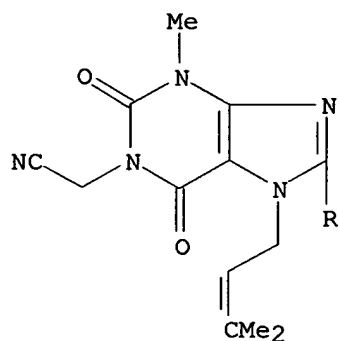
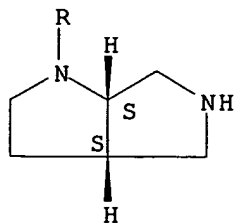
CN 1H-Purine-1-acetonitrile, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-7-(3-methyl-2-butenyl)-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-21-1

CMF C19 H25 N7 O2

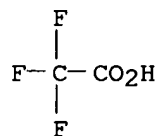
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-24-4 CAPLUS

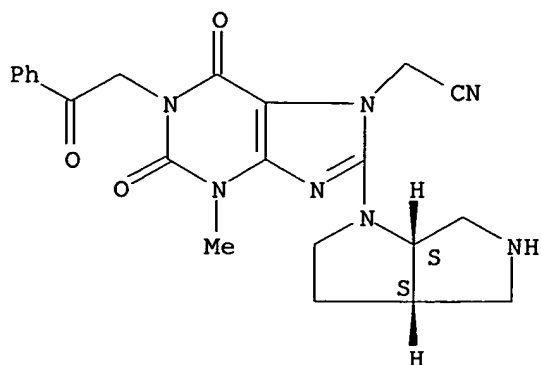
CN 7H-Purine-7-acetonitrile, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-23-3

CMF C22 H23 N7 O3

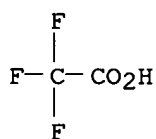
Relative stereochemistry.



CM 2

CRN 76-05-1

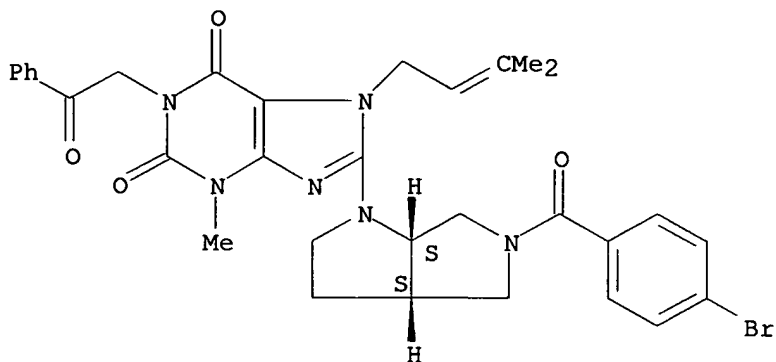
CMF C2 H F3 O2



RN 876130-25-5 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(4-bromobenzoyl)octahydro-1-[2,3,6,7-tetrahydro-3-methyl-7-(3-methyl-2-butenyl)-2,6-dioxo-1-(2-oxo-2-phenylethyl)-1H-purin-8-yl]-, (3aR,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 876130-27-7 CAPLUS

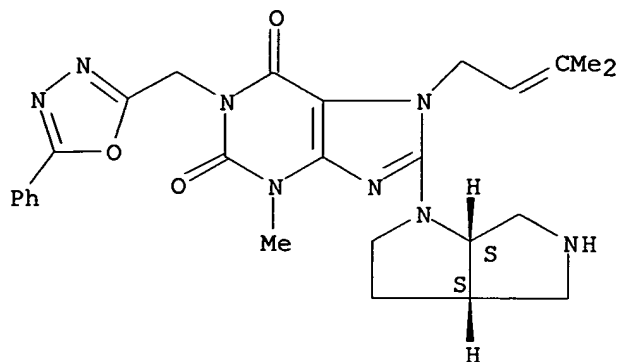
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

10/810,999

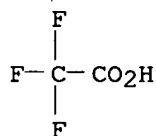
CRN 876130-26-6
CMF C26 H30 N8 O3

Relative stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



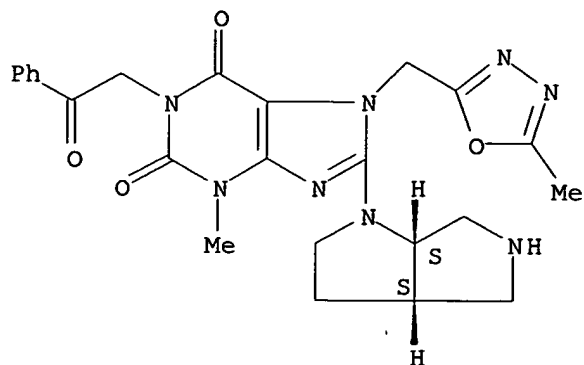
RN 876130-29-9 CAPLUS
CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-[(5-methyl-1,3,4-oxadiazol-2-yl)methyl]-1-(2-oxo-2-phenylethyl)-, rel-, trifluoroacetate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-28-8
CMF C24 H26 N8 O4

Relative stereochemistry.

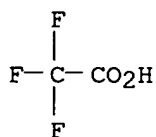
10/810,999



CM 2

CRN 76-05-1

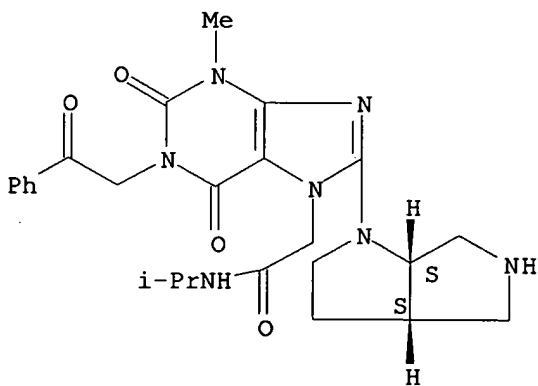
CMF C2 H F3 O2



RN 876130-30-2 CAPLUS

CN 7H-Purine-7-acetamide, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-N-(1-methylethyl)-2,6-dioxo-1-(2-oxo-2-phenylethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



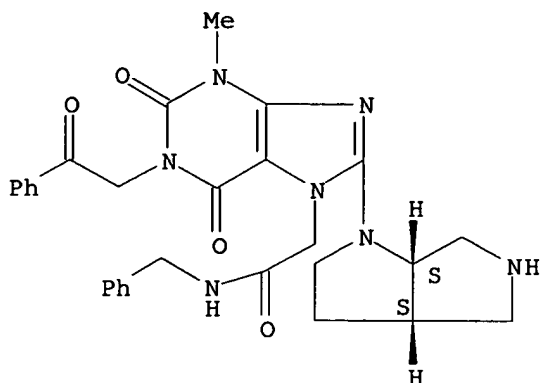
● HCl

RN 876130-31-3 CAPLUS

10/810,999

CN 7H-Purine-7-acetamide, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-N-(phenylmethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

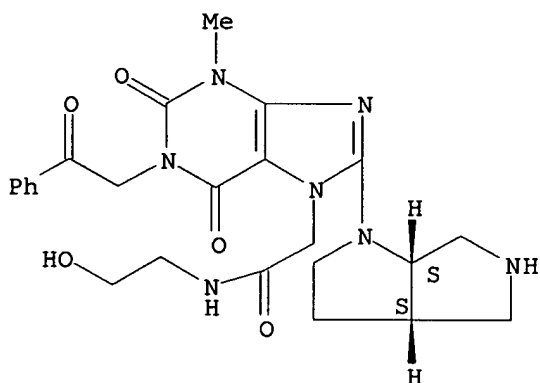


● HCl

RN 876130-32-4 CAPLUS

CN 7H-Purine-7-acetamide, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-N-(2-hydroxyethyl)-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

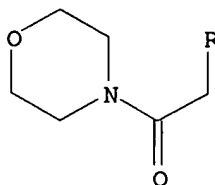
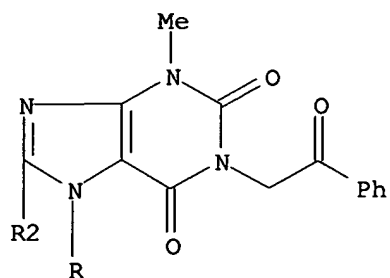
RN 876130-33-5 CAPLUS

CN Morpholine, 4-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-7H-purin-7-yl]acetyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

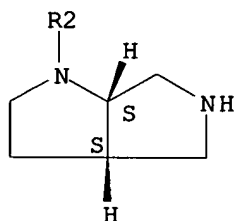
10/810,999

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

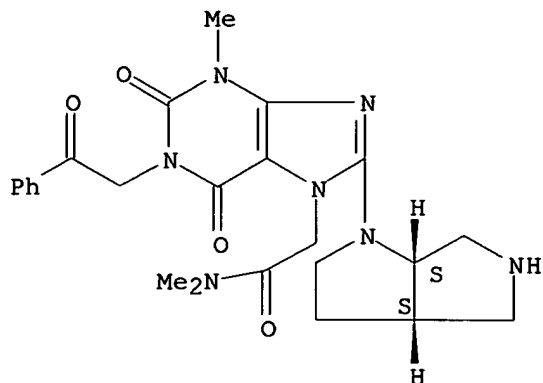


● HCl

RN 876130-34-6 CAPLUS

CN 7H-Purine-7-acetamide, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-N,N,3-trimethyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

RN 876130-36-8 CAPLUS

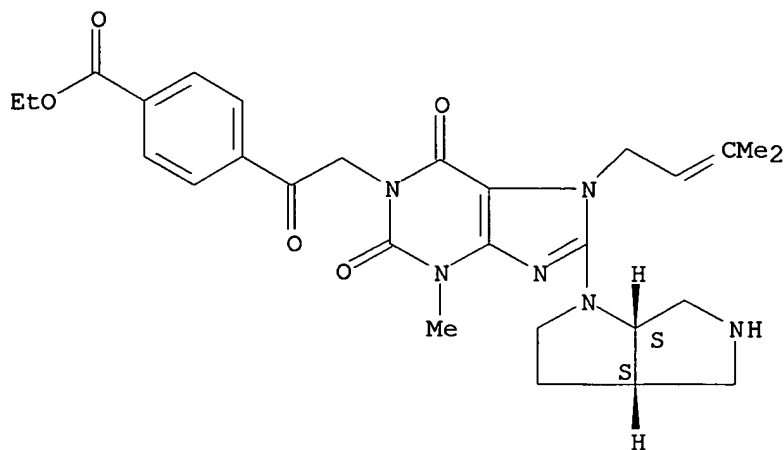
CN Benzoic acid, 4-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-3-methyl-7-(3-methyl-2-butenyl)-2,6-dioxo-1H-purin-1-yl]acetyl]-, ethyl ester, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-35-7

CMF C28 H34 N6 O5

Relative stereochemistry.

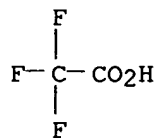


CM 2

CRN 76-05-1

CMF C2 H F3 O2

10/810,999



RN 876130-38-0 CAPLUS

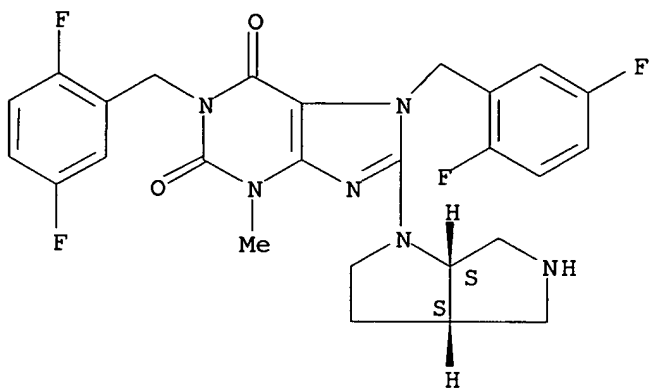
CN 1H-Purine-2,6-dione, 1,7-bis[(2,5-difluorophenyl)methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-37-9

CMF C26 H24 F4 N6 O2

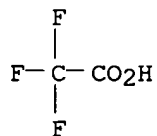
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-40-4 CAPLUS

CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-3-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1-methyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

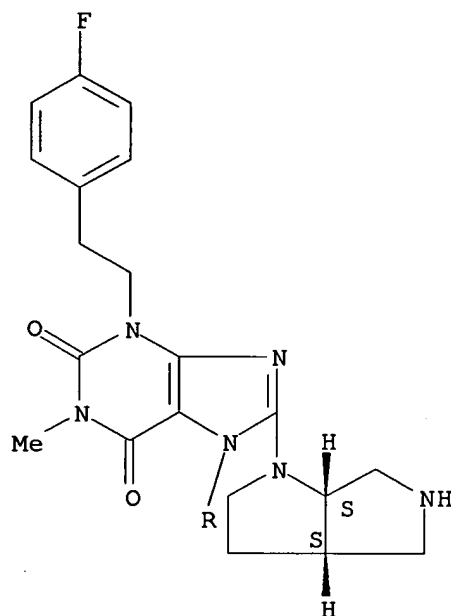
CRN 876130-39-1

10/810,999

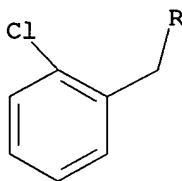
CMF C27 H28 Cl F N6 O2

Relative stereochemistry.

PAGE 1-A



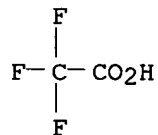
PAGE 2-A



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-42-6 CAPLUS

CN Morpholine, 4-[[7-[(2-chlorophenyl)methyl]-3-[2-(4-fluorophenyl)ethyl]-8-

10/810,999

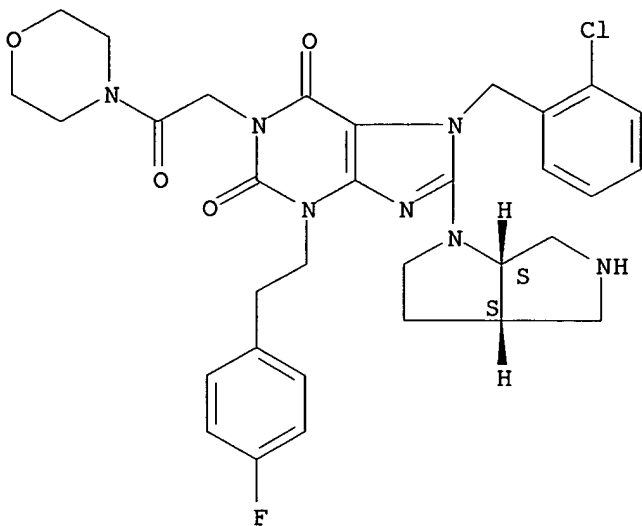
[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-2,6-dioxo-1H-purin-1-yl]acetyl-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-41-5

CMF C32 H35 Cl F N7 O4

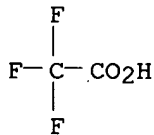
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-44-8 CAPLUS

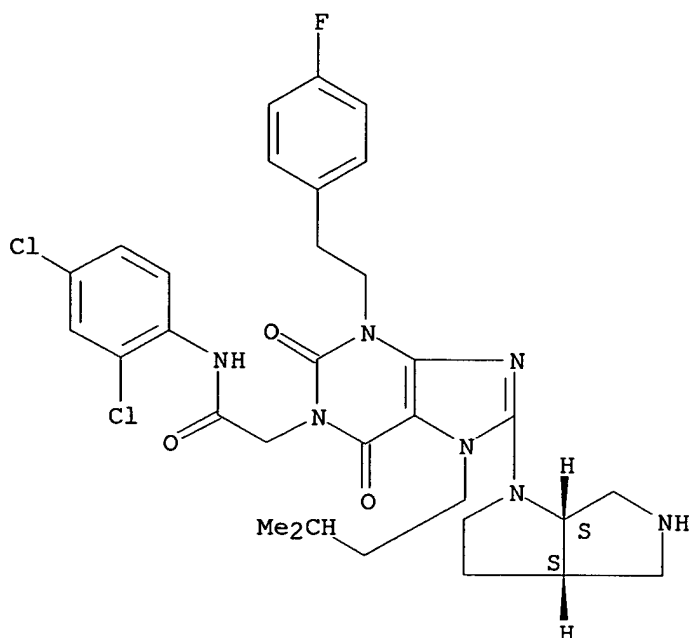
CN 1H-Purine-1-acetamide, N-(2,4-dichlorophenyl)-3-[2-(4-fluorophenyl)ethyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-7-(3-methylbutyl)-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-43-7

CMF C32 H36 Cl2 F N7 O3

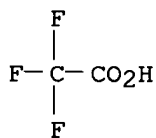
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-46-0 CAPLUS

CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-8-[(3aR,6aR)-
hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-1-methyl-3-(2,2,2-
trifluoroethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

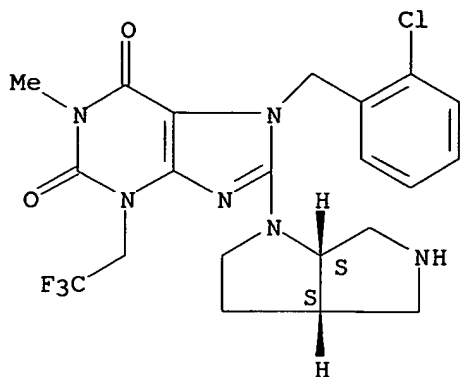
CM 1

CRN 876130-45-9

CMF C21 H22 Cl F3 N6 O2

Relative stereochemistry.

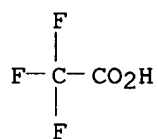
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-48-2 CAPLUS

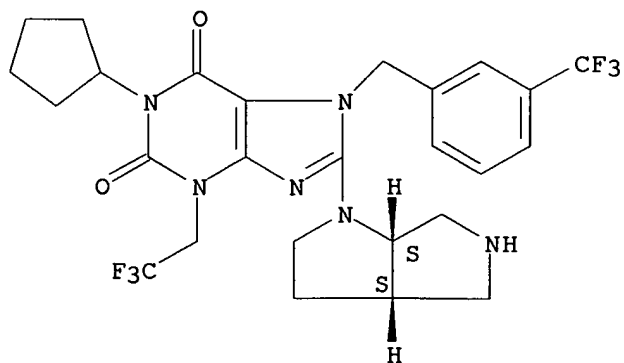
CN 1H-Purine-2,6-dione, 1-cyclopentyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-(2,2,2-trifluoroethyl)-7-[[3-(trifluoromethyl)phenyl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-47-1

CMF C26 H28 F6 N6 O2

Relative stereochemistry.

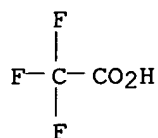


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-50-6 CAPLUS

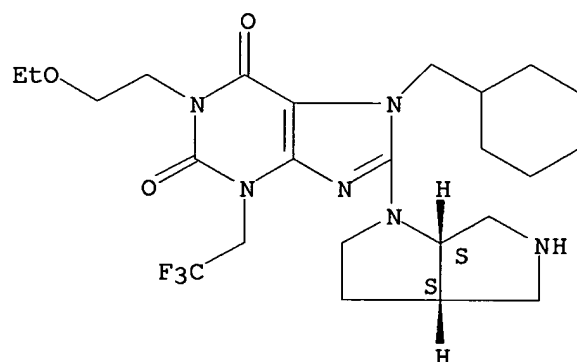
CN 1H-Purine-2,6-dione, 7-(cyclohexylmethyl)-1-(2-ethoxyethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-(2,2,2-trifluoroethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-49-3

CMF C24 H35 F3 N6 O3

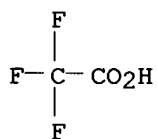
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-52-8 CAPLUS

CN 1H-Purine-1-acetamide, N-(2,4-dichlorophenyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-7-(2-

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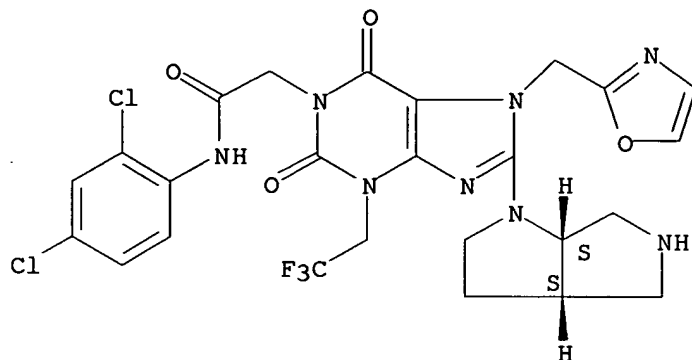
oxazolylmethyl)-2,6-dioxo-3-(2,2,2-trifluoroethyl)-, rel-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-51-7

CMF C25 H23 Cl2 F3 N8 O4

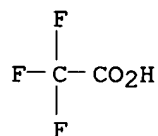
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-54-0 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-
3,7-dihydro-3-methyl-1-(2-oxo-2-phenylethyl)-7-[(2,4,5-
trifluorophenyl)methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX
NAME)

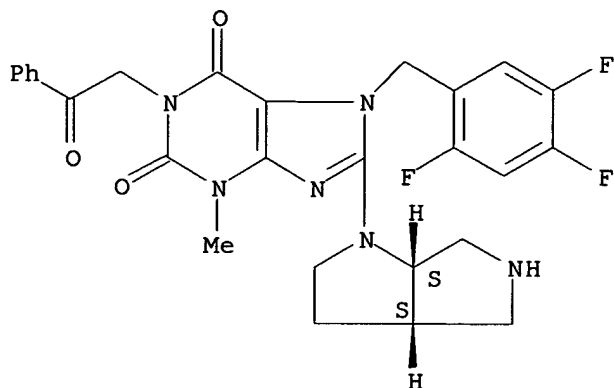
CM 1

CRN 876130-53-9

CMF C27 H25 F3 N6 O3

Relative stereochemistry.

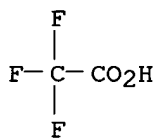
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-56-2 CAPLUS

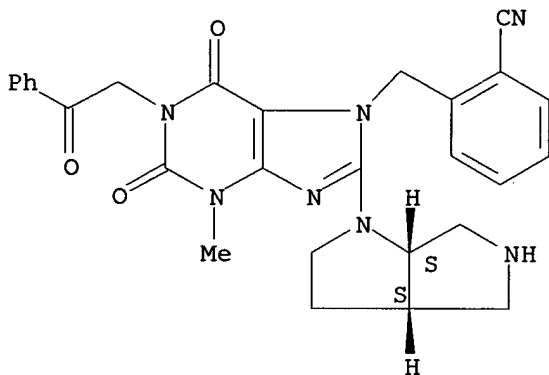
CN Benzonitrile, 2-[[8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-1-(2-oxo-2-phenylethyl)-7H-purin-7-yl]methyl]-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-55-1

CMF C28 H27 N7 O3

Relative stereochemistry.

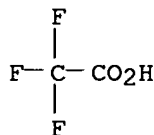


10/810,999

CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-58-4 CAPLUS

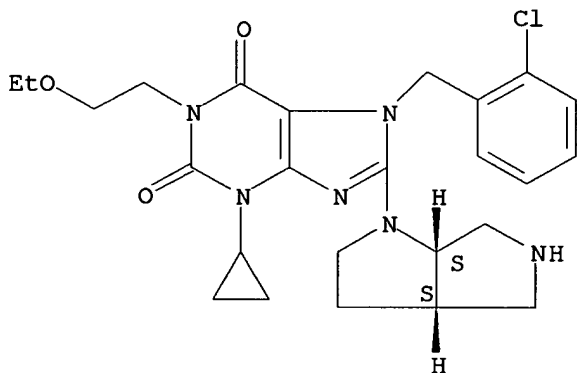
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-3-cyclopropyl-1-(2-ethoxyethyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-57-3

CMF C25 H31 Cl N6 O3

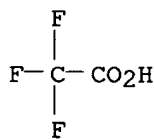
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-60-8 CAPLUS

CN 1H-Purine-2,6-dione, 3-cyclopropyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-7-(3-methylbutyl)-1-(2-oxo-2-

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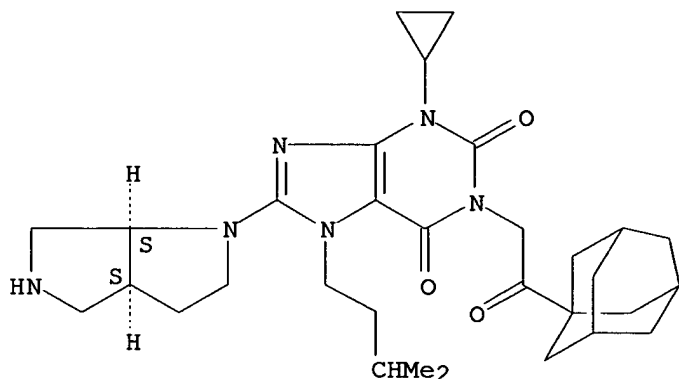
tricyclo[3.3.1.1^{3,7}]dec-1-ylethyl)-, rel-, mono(trifluoroacetate) (9CI)
(CA INDEX NAME)

CM 1

CRN 876130-59-5

CMF C31 H44 N6 O3

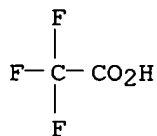
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-62-0 CAPLUS

CN 1H-Purine-1-acetamide, 3-cyclopropyl-N-(2,4-dichlorophenyl)-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2,3,6,7-tetrahydro-7-(2-oxazolylmethyl)-2,6-dioxo-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

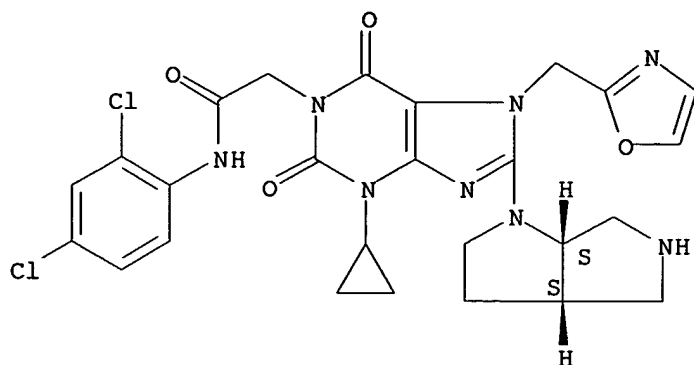
CM 1

CRN 876130-61-9

CMF C26 H26 Cl2 N8 O4

Relative stereochemistry.

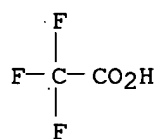
10/810,999



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 876130-64-2 CAPLUS

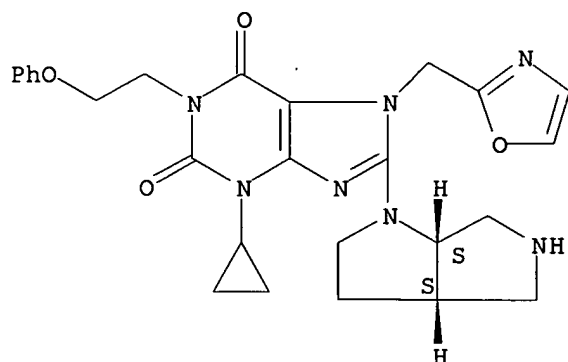
CN 1H-Purine-2,6-dione, 3-cyclopropyl-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-7-(2-oxazolylmethyl)-1-(2-phenoxyethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 876130-63-1

CMF C26 H29 N7 O4

Relative stereochemistry.

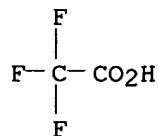


10/810,999

CM 2

CRN 76-05-1

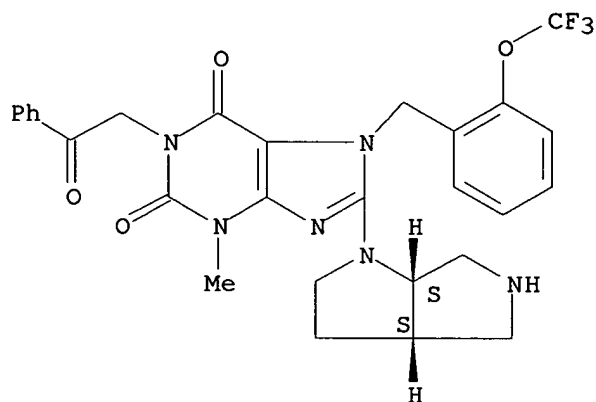
CMF C2 H F3 O2



RN 876130-65-3 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-phenylethyl)-7-[[2-(trifluoromethoxy)phenyl]methyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

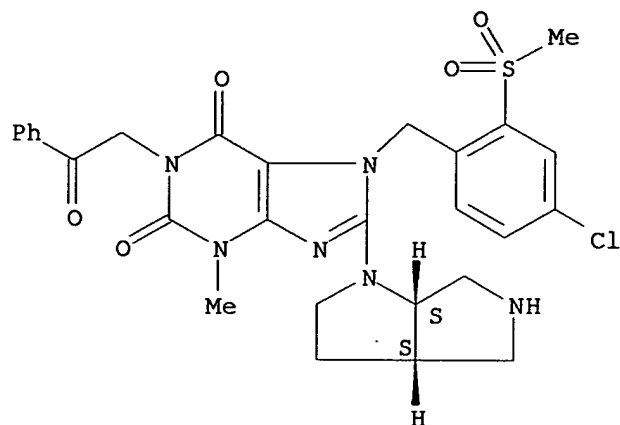


● HCl

RN 876130-66-4 CAPLUS

CN 1H-Purine-2,6-dione, 7-[[4-chloro-2-(methylsulfonyl)phenyl]methyl]-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-1-(2-oxo-2-phenylethyl)-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

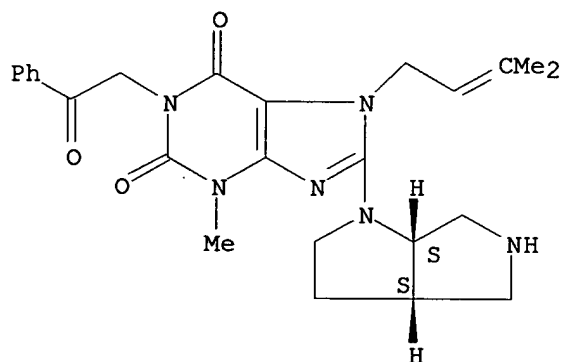


● HCl

RN 876130-67-5 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

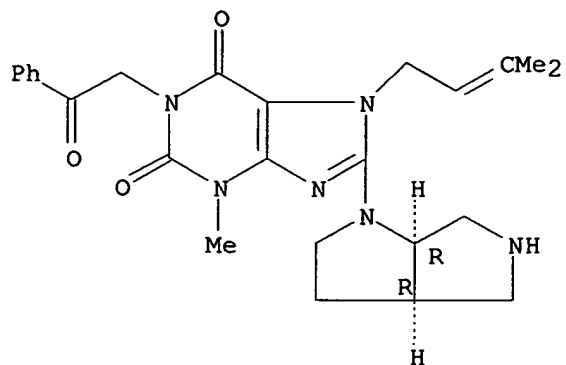


● HCl

RN 876130-68-6 CAPLUS

CN 1H-Purine-2,6-dione, 8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-1-(2-oxo-2-phenylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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~~L10~~ ANSWER 3 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:409230 CAPLUS

DOCUMENT NUMBER: 142:463912

TITLE: Substituted diazabicycloalkane derivatives

INVENTOR(S): Basha, Anwer; Bunnelle, William H.; Dart, Michael J.;
Gallagher, Megan E.; Ji, Jianguo; Li, Tao; Pace,
Jennifer M.; Ryther, Keith B.; Tietje, Karin R.;
Mortell, Kathleen H.; Nersesian, Diana L.; Schrimpf,
Michael R.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 92 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005101602	A1	20050512	US 2004-942035	20040916
PRIORITY APPLN. INFO.:			US 2003-504353P	P 20030919
OTHER SOURCE(S):	MARPAT 142:463912			

AB Compds. of formula Z-Ar1-Ar2 (Z = diazabicyclic amine, Ar1 is a 5- or 6-membered aromatic ring, and Ar2 is selected from the group consisting of an unsubstituted or substituted 5- or 6-membered heteroaryl ring; unsubstituted or substituted bicyclic heteroaryl ring; 3,4-(methylenedioxy)phenyl; carbazoyl; tetrahydrocarbazoyl; naphthyl; and phenyl; wherein the Ph is substituted with 0, 1, 2, or 3 substituents in the meta- or para-positions). The compds. are useful in treating conditions or disorders prevented by or ameliorated by nAChR ligands.

IT **851521-82-9P 851524-11-3P**

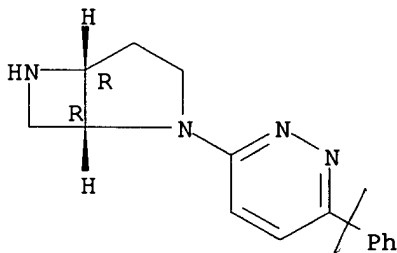
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted diazabicycloalkane derivs. for the treatment of disorders prevented by or ameliorated by nAChR ligands)

RN 851521-82-9 CAPLUS

CN 2,6-Diazabicyclo[3.2.0]heptane, 2-(6-phenyl-3-pyridazinyl)-, (1R,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 851524-11-3 CAPLUS

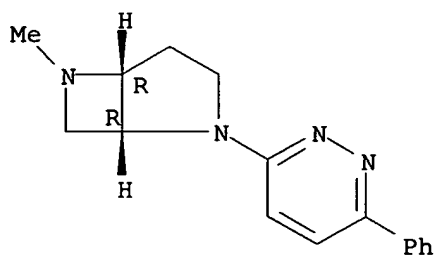
CN 2,6-Diazabicyclo[3.2.0]heptane, 6-methyl-2-(6-phenyl-3-pyridazinyl)-, (1R,5R)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

10/810,999

CRN 851524-10-2
CMF C16 H18 N4

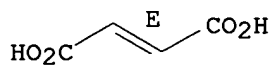
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



10/810,999

100 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:394825 CAPLUS

DOCUMENT NUMBER: 142:430293

TITLE: Preparation of quinazolinyl norepinephrine reuptake inhibitors for the treatment of central nervous system disorders

INVENTOR(S): Caprathe, Bradley William; Glase, Shelly Ann; Konstantinou, Zissis; Schelkun, Robert Michael; Sheehan, Susan M.; Thomas, Anthony Jerome; Yuen, Po-wai

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 44 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

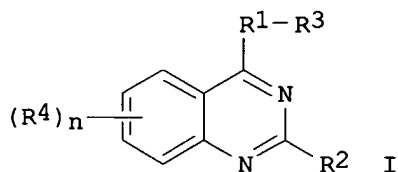
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005096327	A1	20050505	US 2004-979651	20041102
WO 2005042501	A1	20050512	WO 2004-IB3535	20041026
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: US 2003-516879P P 20031103
US 2004-611292P P 20040921

OTHER SOURCE(S): MARPAT 142:430293

GI



AB Title compds. I [R1 = alkyl, cycloalkyl, alkoxy, etc.; R2 = alkyl, cycloalkyl, amino, etc.; R3 = H, (cyclo)alkyl, etc.; R4 = H, halo, NO2, etc.] are prepared For instance, 2-(4-methylpiperazin-1-yl)-4-phenylquinazoline (II) is prepared in 3 steps from 2-aminobenzophenone, urea and 1-methylpiperazine. II has Ki = 29.7 nM for the norepinephrine transporter receptor. I are useful for the treatment of central nervous system disorders.

IT **851013-92-8P 851014-66-9P**, 4-(2,4-Difluorophenyl)-7-fluoro-2-(hexahydropyrrolo[3,4-b]pyrrol-1-yl)quinazoline
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

10/810,999

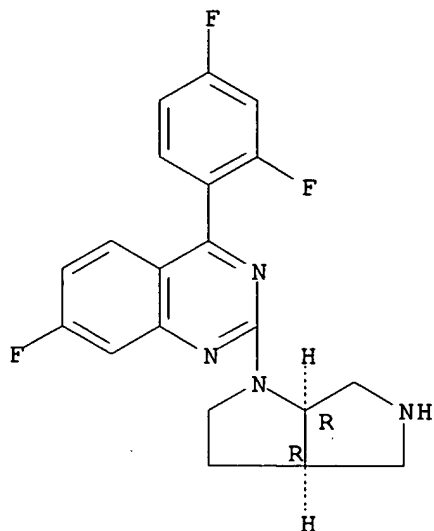
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinazolinyl norepinephrine reuptake inhibitors for treatment of central nervous system disorders)

RN 851013-92-8 CAPLUS

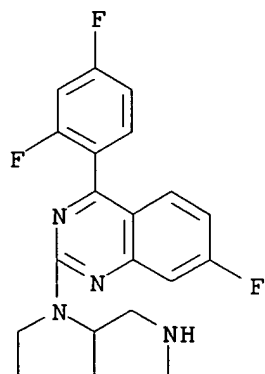
CN Quinazoline, 4-(2,4-difluorophenyl)-7-fluoro-2-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 851014-66-9 CAPLUS

CN Quinazoline, 4-(2,4-difluorophenyl)-7-fluoro-2-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)- (9CI) (CA INDEX NAME)



10/810,999

110 ANSWER 5 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:902383 CAPLUS

DOCUMENT NUMBER: 141:379947

TITLE: Preparation of triazolotriazines and related derivatives as A2a adenosine receptor antagonists
INVENTOR(S): Peng, Hairuo; Yao, Gang; Vu, Chi; Petter, Russell C.; Kumaravel, Gnanasambandam

PATENT ASSIGNEE(S): Biogen Idec Ma Inc., USA

SOURCE: PCT Int. Appl., 80 pp.

CODEN: PIXXD2

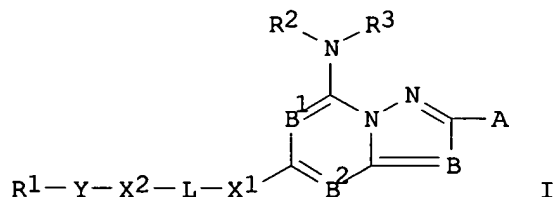
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092173	A2	20041028	WO 2004-US11009	20040409
WO 2004092173	A3	20041209		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1633756	A2	20060315	EP 2004-759359	20040409
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
PRIORITY APPLN. INFO.:			US 2003-461484P	P 20030409
			WO 2004-US11009	W 20040409
OTHER SOURCE(S):	MARPAT 141:379947			
GI				



AB Title compds. I [A = (hetero)aryl; B, B1-2 = N, CR2, provided at least on B1 or B2 is N; R2-3 = H, alkyl, cycloalkyl, etc.; X1 = bond, alkylene, alkenylene, etc.; X2 = bond, alkylene, alkenylene, etc.; L = linker, e.g., bridged bicyclic diazo-substituted carbocyclic ring, etc.; Y = alkyl, amino, etc.] are prepared For instance, cis-[2-(7-amino-2-(furan-2-yl)-[1,2,4]triazolo[1,5-a]triazin-5-yl)octahydropyrido[1,2-a]pyrazin-7-yl]methanol is prepared from 2-(furan-2-yl)-5-methanesulfonyl-

[1,2,4]triazolo[1,5-a][1,3,5]triazin-7-ylamine and [octahydroxyrido[1,2-a]pyrazin-7-yl]methanol. Compds. I exhibit $K_i < 10 \mu\text{M}$ for the A2a receptor. I are useful in treating Parkinson's disease.

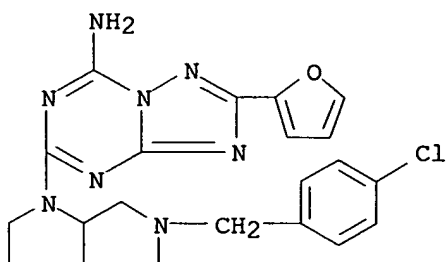
IT **781638-76-4P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of triazolotriazines and related derivs. as A2a adenosine receptor antagonists for the treatment of, e.g., Parkinson's disease)

RN 781638-76-4 CAPLUS

CN [1,2,4]Triazolo[1,5-a][1,3,5]triazin-7-amine, 5-[5-[(4-chlorophenyl)methyl]hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-2-(2-furanyl)-(9CI) (CA INDEX NAME)



10/810,999

L10 ANSWER 6 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:390240 CAPLUS

DOCUMENT NUMBER: 140:406815

TITLE: Preparation of phenylaminopyrimidines as Rho-Kinase II (ROK α) inhibitors for the treatment of cardiovascular diseases.

INVENTOR(S): Feurer, Achim; Bennabi, Samir; Heckroth, Heike; Schirok, Hartmut; Mittendorf, Joachim; Kast, Raimund; Stasch, Johannes-peter; Gnoth, Mark Jean; Muentner, Klaus; Lang, Dieter; Figueroa, Perez Santiago; Ehmke, Heimo

PATENT ASSIGNEE(S): Bayer Healthcare Ag, Germany; et al.

SOURCE: PCT Int. Appl., 203 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

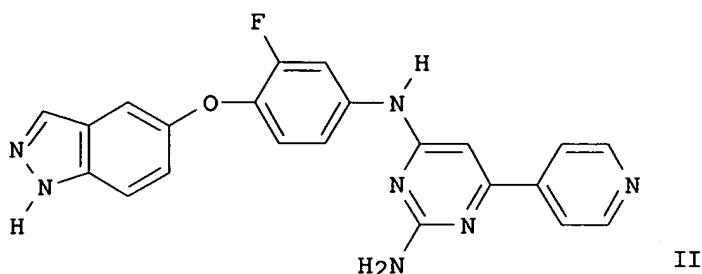
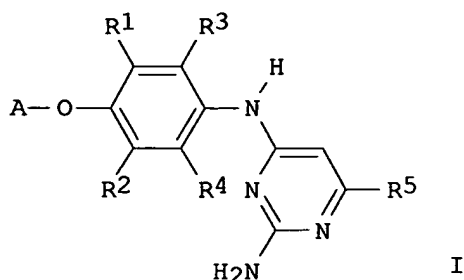
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039796	A1	20040513	WO 2003-EP11452	20031016
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10332232	A1	20040513	DE 2003-10332232	20030716
CA 2503646	AA	20040513	CA 2003-2503646	20031016
AU 2003278088	A1	20040525	AU 2003-278088	20031016
EP 1562935	A1	20050817	EP 2003-769398	20031016
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006506458	T2	20060223	JP 2005-501803	20031016
PRIORITY APPLN. INFO.:			DE 2002-10250113	A 20021028
			DE 2003-10332232	A 20030716
			WO 2003-EP11452	W 20031016

OTHER SOURCE(S): MARPAT 140:406815

GI



AB Title compds. I [A = (un)substituted indazole, dihydrobenzofuran, indoline, etc.: R1 = H, halo, CN; R3, R4 = H, F, Cl; R5 = H, OH, halo, etc.] and their pharmaceutically acceptable salts were prepared. For example, condensation of 5-(4-amino-2-fluorophenoxy)-1H-indazol, e.g., prepared from 5-hydroxyindazole in 2-steps, and 4-chloro-6-(4-pyridinyl)-2-pyrimidinamine, e.g., prepared from isonicotinic acid in 3-steps, afforded phenylaminopyrimidine II in 62% yield. In Rho-Kinase II (ROK α) inhibition assays, 13-examples of compds. I exhibited IC50 values ranging from 1-680 nM, e.g., the IC50 value of phenylaminopyrimidine II was 20 nM. Compds. I were claimed useful for the treatment of cardiovascular diseases.

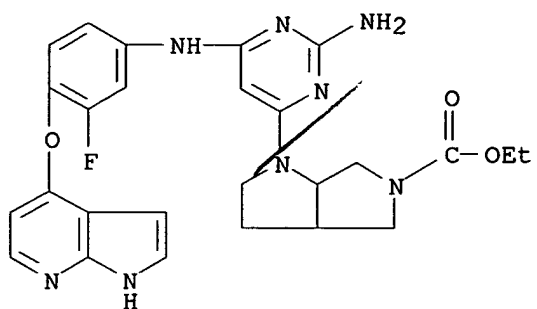
IT **688780-43-0P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phenylaminopyrimidines as Rho-Kinase II (ROK α) inhibitors for the treatment of cardiovascular diseases)

RN 688780-43-0 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, 1-[2-amino-6-[[3-fluoro-4-(1H-pyrrolo[2,3-b]pyridin-4-yloxy)phenyl]amino]-4-pyrimidinyl]hexahydro-, ethyl ester (9CI) (CA INDEX NAME)



10/810,999

~~110~~ ANSWER 7 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:370934 CAPLUS

DOCUMENT NUMBER: 140:391293

TITLE: Preparation of purines as cannabinoid receptor ligands (CB-1 receptor antagonists).

INVENTOR(S): Griffith, David Andrew

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 191 pp.

CODEN: PIXXD2

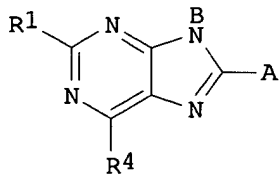
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037823	A1	20040506	WO 2003-IB4619	20031021
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004092520	A1	20040513	US 2003-689381	20031020
CA 2503900	AA	20040506	CA 2003-2503900	20031021
AU 2003269368	A1	20040513	AU 2003-269368	20031021
BR 2003014918	A	20050802	BR 2003-14918	20031021
EP 1558615	A1	20050803	EP 2003-751149	20031021
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006505581	T2	20060216	JP 2004-546275	20031021
NL 1024643	A1	20040503	NL 2003-1024643	20031028
NL 1024643	C2	20050201		
NO 2005002512	A	20050525	NO 2005-2512	20050525
PRIORITY APPLN. INFO.:			US 2002-421874P	P 20021028
			WO 2003-IB4619	W 20031021
OTHER SOURCE(S):	MARPAT 140:391293			
GI				



I

AB Title compds. [I; A, B = (substituted) aryl, heteroaryl; R1 = H, alkyl, haloalkyl, alkoxy; R4 = specified (substituted) alkoxy, cycloalkoxy, N-heterocyclyl, etc.], were prepared Thus, 6-chloro-9-(4-chlorophenyl)-8-(2,4-dichlorophenyl)-9H-purine (preparation given) was added to a mixture prepared

from Na and Me₂CHOH followed by stirring at room temperature overnight to give 26% 9-(4-chlorophenyl)-8-(2,4-dichlorophenyl)-6-isopropoxy-9H-purine. In a CB-1 receptor binding assay, I showed binding activities in the range of 0.17 nM to 1 μ M.

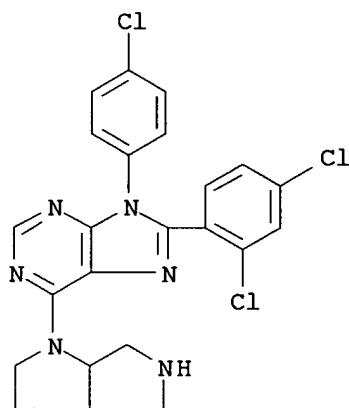
IT **686346-10-1P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of purines as cannabinoid receptor ligands (CB-1 receptor antagonists))

RN 686346-10-1 CAPLUS

CN 9H-Purine, 9-(4-chlorophenyl)-8-(2,4-dichlorophenyl)-6-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)- (9CI) (CA INDEX NAME)



10/810,999

L10 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:80686 CAPLUS

DOCUMENT NUMBER: 140:146157

TITLE: Preparation of pyrazolopyridinylpyrimidines as inhibitors of cGMP degradation for the treatment of central nervous system diseases

INVENTOR(S): Feurer, Achim; Luithle, Joachim; Wirtz, Stephan-nicholas; Koenig, Gerhard; Stasch, Johannes-peter; Stahl, Elke; Schreiber, Rudy; Wunder, Frank; Lang, Dieter

PATENT ASSIGNEE(S): Bayer Healthcare Ag, Germany

SOURCE: PCT Int. Appl., 96 pp.

CODEN: PIXXD2

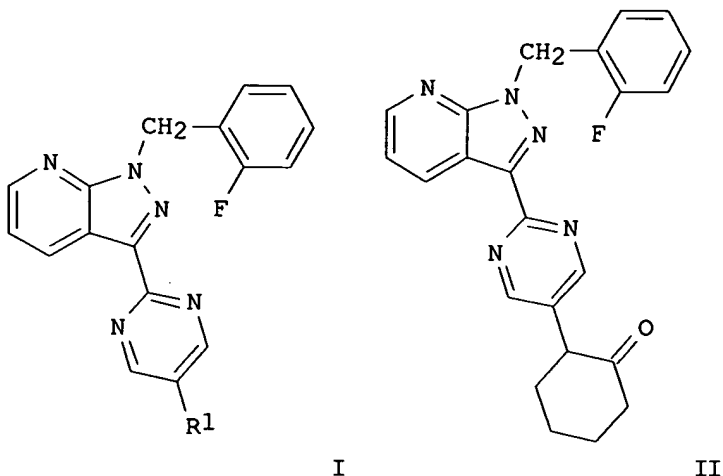
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009589	A1	20040129	WO 2003-EP7238	20030707
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10232572	A1	20040205	DE 2002-10232572	20020718
CA 2492723	AA	20040129	CA 2003-2492723	20030707
AU 2003257437	A1	20040209	AU 2003-257437	20030707
EP 1525202	A1	20050427	EP 2003-764943	20030707
EP 1525202	B1	20060111		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006502119	T2	20060119	JP 2004-522411	20030707
PRIORITY APPLN. INFO.:			DE 2002-10232572	A 20020718
			WO 2003-EP7238	W 20030707
OTHER SOURCE(S):	MARPAT 140:146157			
GI				

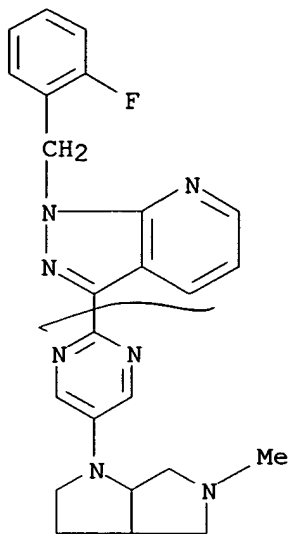


AB Title compds. I [R1 = (un)substituted aryl, heteroaryl, benzodioxole, etc.] and their pharmaceutically acceptable salts were prepared For example, palladium mediated coupling of bromide I [R1 = Br], e.g., prepared from 2-fluorobenzylhydrazine in 6-steps, and cyclohexanone afforded pyrazolopyridinylpyrimidine II in 29% yield. In cGMP degradation inhibition assays, 10-examples of compds. I exhibited a significant increase (sic) in cGMP concentration at 0.27-1.2 μ M inhibitor concentration Compds. I are claimed

IT **651339-82-1P**
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (target compound; preparation of pyrazolopyridinylpyrimidines as inhibitors of cGMP degradation for the treatment of central nervous system diseases)

RN 651339-82-1 CAPLUS

CN 1H-Pyrazolo[3,4-b]pyridine, 1-[(2-fluorophenyl)methyl]-3-[5-(hexahydro-5-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/810,999

~~L10~~ ANSWER 9 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:1006976 CAPLUS

DOCUMENT NUMBER: 140:59653

TITLE: Preparation of phenylaminopyrimidines as rho-kinase inhibitors

INVENTOR(S): Feurer, Achim; Bennabi, Samir; Heckroth, Heike; Ergueden, Jens; Schenke, Thomas; Bauser, Markus; Kast, Raimund; Stasch, Johannes-Peter; Stahl, Elke; Muentner, Klaus; Lang, Dieter; Ehmke, Heimo

PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

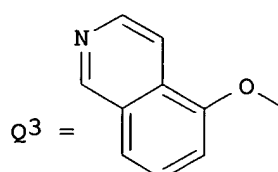
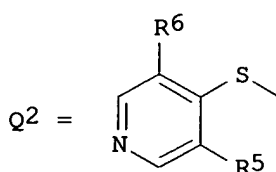
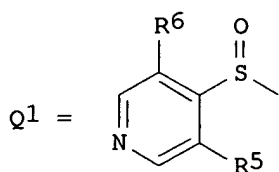
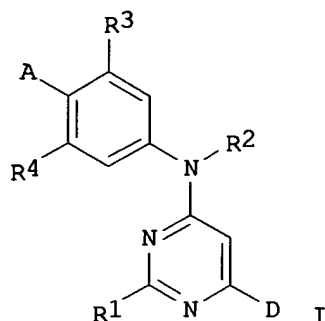
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003106450	A1	20031224	WO 2003-EP5827	20030604
WO 2003106450	C1	20050203		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
DE 10226943	A1	20040108	DE 2002-10226943	20020617
CA 2489452	AA	20031224	CA 2003-2489452	20030604
AU 2003232848	A1	20031231	AU 2003-232848	20030604
EP 1515965	A1	20050323	EP 2003-759908	20030604
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 2005538962	T2	20051222	JP 2004-513282	20030604
PRIORITY APPLN. INFO.:			DE 2002-10226943	A 20020617
			WO 2003-EP5827	W 20030604
OTHER SOURCE(S):	MARPAT 140:59653			
GI				



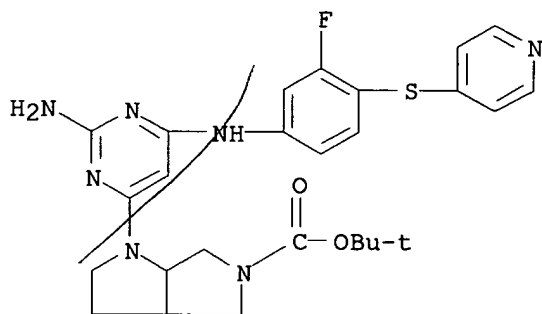
AB Title compds. [I; R1 = amino, OH; R2 = H, alkyl, cycloalkyl; R3, R4 = cyano, H, F, Cl; A = Q1-Q3; R5, R6 = H, F, Cl; D = (substituted) Ph, (iso)quinoline, indole, etc.], were prepared for treating cardiovascular diseases. Thus, 4-chloro-6-quinolin-6-yl-pyrimidin-2-amine (preparation given) and 3-fluoro-4-(4-pyridinylsulfanyl)aniline (preparation given) were treated with 37% HCl followed by stirring for over night at 100° to give 12% N-[2-amino-6-(6-quinolinyl)-4-pyrimidinyl]-N-[3-fluoro-4-(4-pyridinylsulfanyl)phenyl]amine. The latter inhibited Rho-kinase II (ROK α) with IC₅₀ = 7 nM.

IT **637039-59-9P 637039-82-8P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of phenylaminopyrimidines as rho-kinase inhibitors)

RN 637039-59-9 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, 1-[2-amino-6-[[3-fluoro-4-(4-pyridinylthio)phenyl]amino]-4-pyrimidinyl]hexahydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



10/810,999

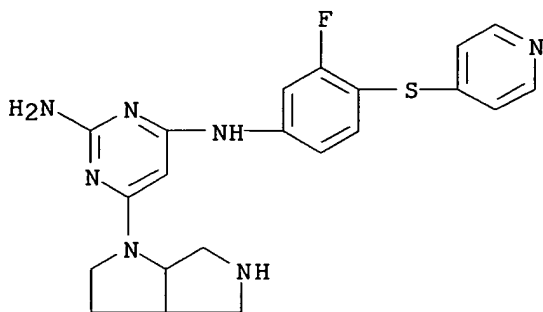
RN 637039-82-8 CAPLUS

CN 2,4-Pyrimidinediamine, N4-[3-fluoro-4-(4-pyridinylthio)phenyl]-6-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 637039-81-7

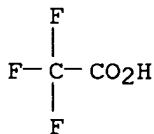
CMF C21 H22 F N7 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



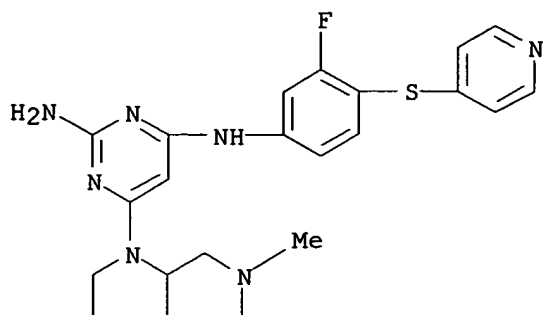
IT 637039-30-6P 637039-81-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phenylaminopyrimidines as rho-kinase inhibitors)

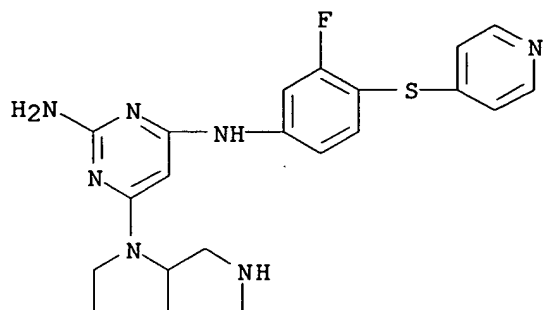
RN 637039-30-6 CAPLUS

CN 2,4-Pyrimidinediamine, N4-[3-fluoro-4-(4-pyridinylthio)phenyl]-6-(hexahydro-5-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl)- (9CI) (CA INDEX NAME)



RN 637039-81-7 CAPLUS

CN 2,4-Pyrimidinediamine, N4-[3-fluoro-4-(4-pyridinylthio)phenyl]-6-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/810,999

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L10 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:784071 CAPLUS

DOCUMENT NUMBER: 140:12454

TITLE: Design and synthesis of pyrrolidine-5,5'-trans-lactams (5-oxo-hexahydropyrrolo[3,2-b]pyrroles) as novel mechanism-based inhibitors of human cytomegalovirus protease. 4. Antiviral activity and plasma stability

AUTHOR(S): Borthwick, Alan D.; Davies, Dave E.; Ertl, Peter F.; Exall, Anne M.; Haley, Terry M.; Hart, Graham J.; Jackson, Deborah L.; Parry, Nigel R.; Patikis, Angela; Trivedi, Naimisha; Weingarten, Gordon G.; Woolven, James M.

CORPORATE SOURCE: Department of Medicinal Chemistry CVU UK, Medicines Research Centre, GlaxoSmithKline Research and Development, Herts, SG1 2NY, UK

SOURCE: Journal of Medicinal Chemistry (2003), 46(21), 4428-4449

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:12454

AB A series of chiral, (S)-proline- α -methylpyrrolidine-5,5-trans-lactam serine protease inhibitors has been developed as antivirals of human cytomegalovirus (HCMV). The SAR of the functionality on the proline nitrogen has shown that derivs. of para-substituted Ph ureas > para-substituted Ph sulfonamides > para-substituted Ph carboxamide for activity against HCMV δ Ala protease, producing para-substituted Ph ureas with single figure nM potency (K_i) against the viral enzyme. The SAR of the functionality on the lactam nitrogen has defined the steric and electronic requirements for high human plasma stability while retaining good activity against HCMV protease. The combination of high potency against HCMV δ Ala protease and high human plasma stability has produced compds. with significant in vitro antiviral activity against human cytomegalovirus with the 6-hydroxymethyl benzothiazole derivative 72 being equivalent in potency to ganciclovir. The parent benzothiazole 56 had good pharmacokinetics in dogs with 29% bioavailability and good brain and ocular penetration in guinea pigs.

IT 214336-71-7P

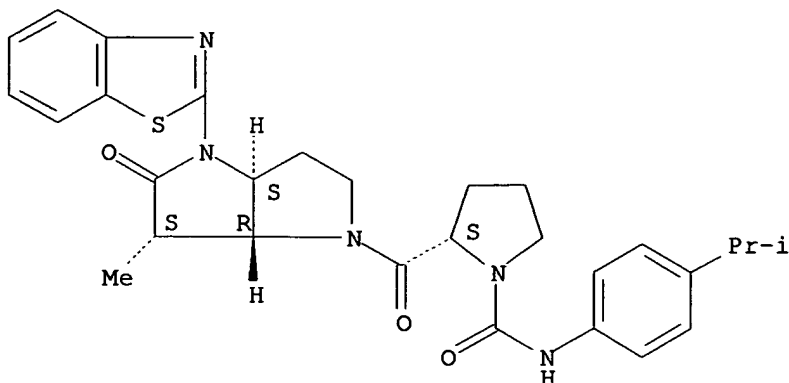
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and antiviral structure activity relationships of pyrrolidine-lactams as inhibitors of human cytomegalovirus protease)

RN 214336-71-7 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 214336-74-0P 214336-75-1P 214336-76-2P
 214336-77-3P 214336-80-8P 214336-81-9P
 214336-82-0P 214336-83-1P 214336-90-0P
 214337-65-2P 214337-66-3P 214337-68-5P
 628725-94-0P 628725-95-1P 628725-96-2P

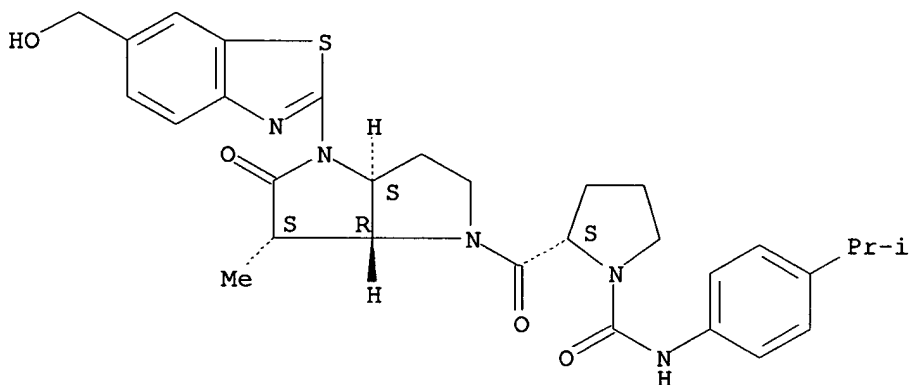
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and antiviral structure activity relationships of pyrrolidine-lactams as inhibitors of human cytomegalovirus protease)

RN 214336-74-0 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-hexahydro-4-[6-(hydroxymethyl)-2-benzothiazolyl]-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

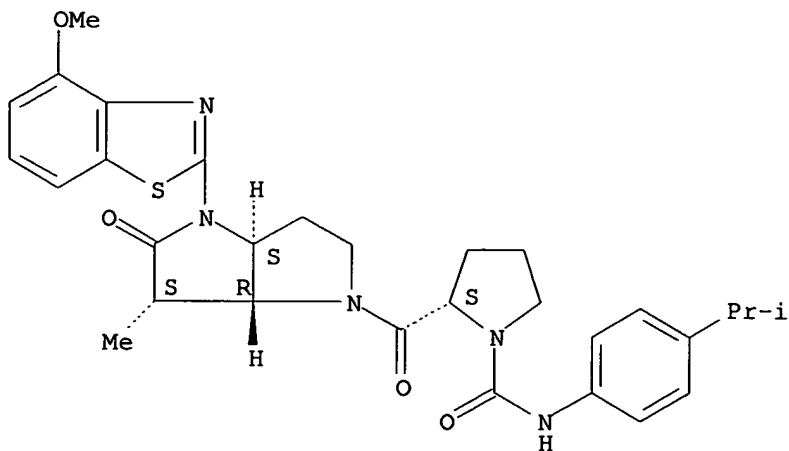
Absolute stereochemistry.



RN 214336-75-1 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aS)-hexahydro-4-(4-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

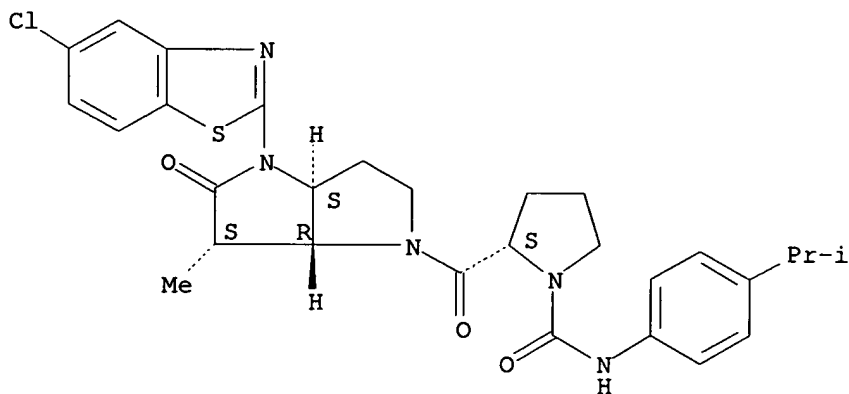
Absolute stereochemistry.



RN 214336-76-2 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-4-(5-chloro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

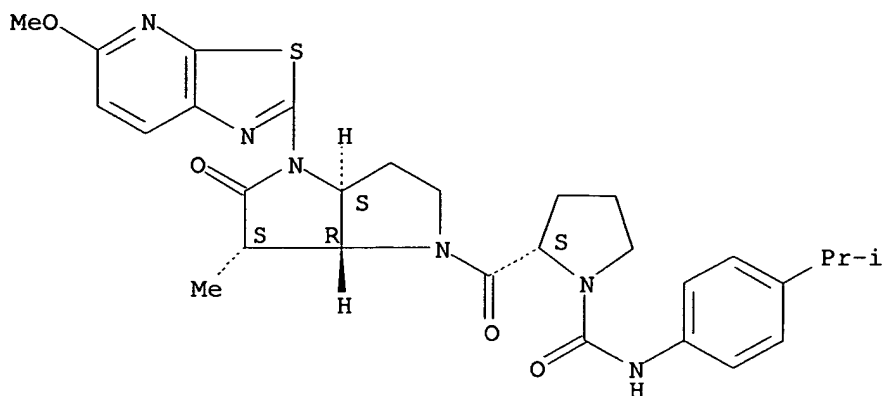
Absolute stereochemistry.



RN 214336-77-3 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-4-(5-methoxythiazolo[5,4-b]pyridin-2-yl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

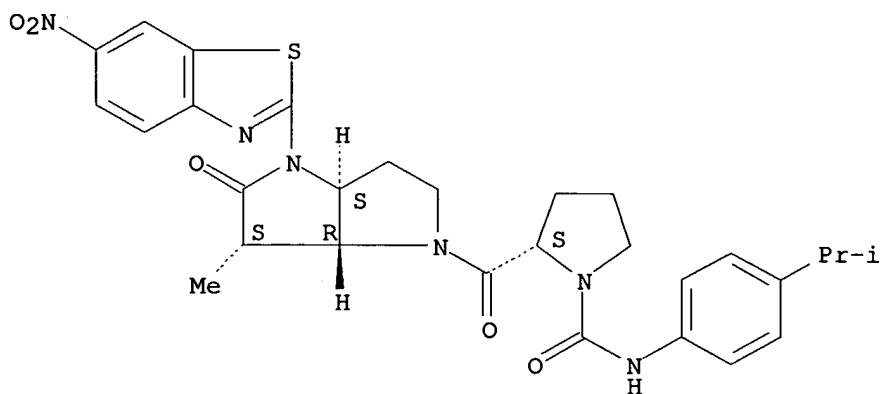
Absolute stereochemistry.



RN 214336-80-8 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-6-methyl-4-(6-nitro-2-benzothiazolyl)-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

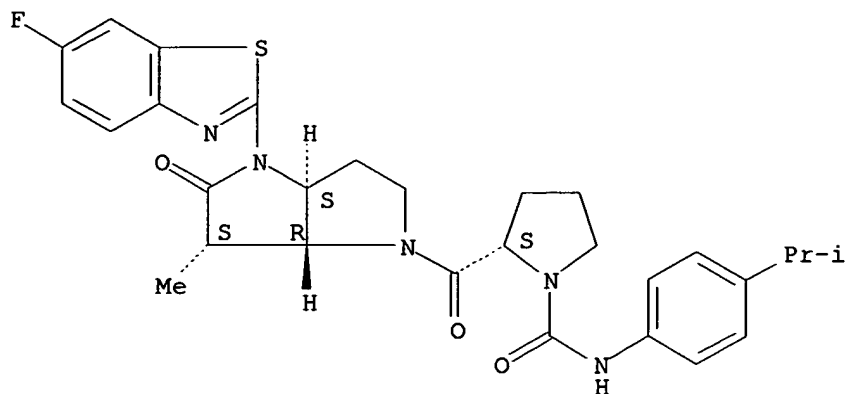
Absolute stereochemistry.



RN 214336-81-9 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-4-(6-fluoro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

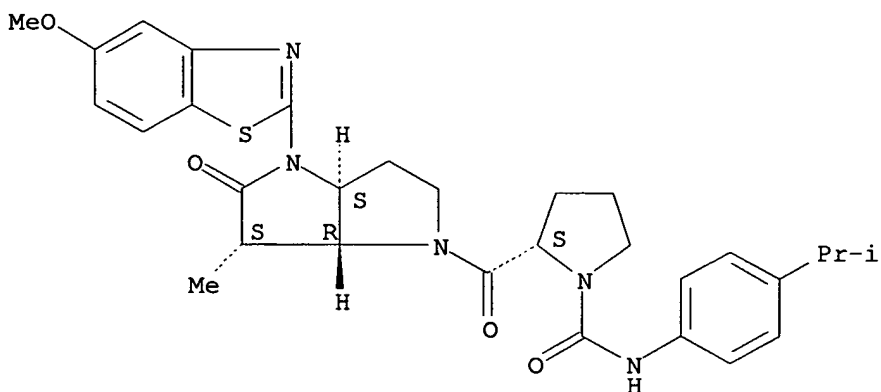
Absolute stereochemistry.



RN 214336-82-0 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-4-(5-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

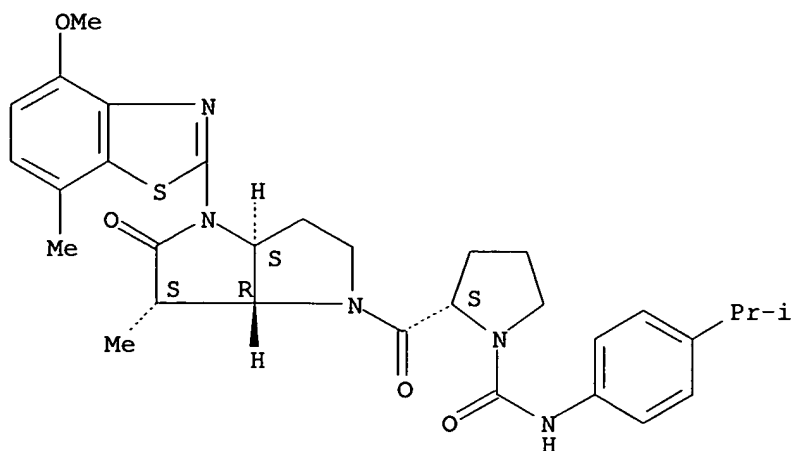
Absolute stereochemistry.



RN 214336-83-1 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-4-(4-methoxy-7-methyl-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

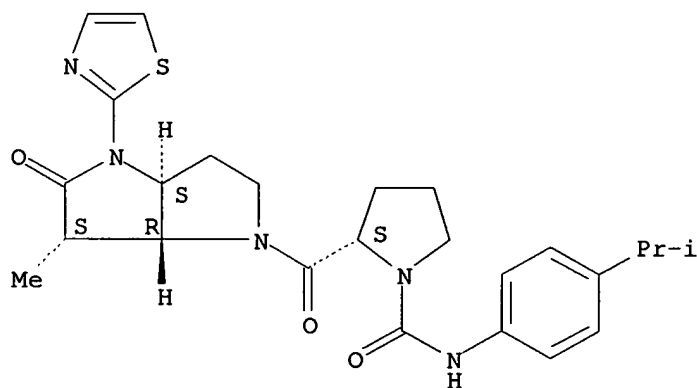
Absolute stereochemistry.



RN 214336-90-0 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-(2-methylethyl)pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

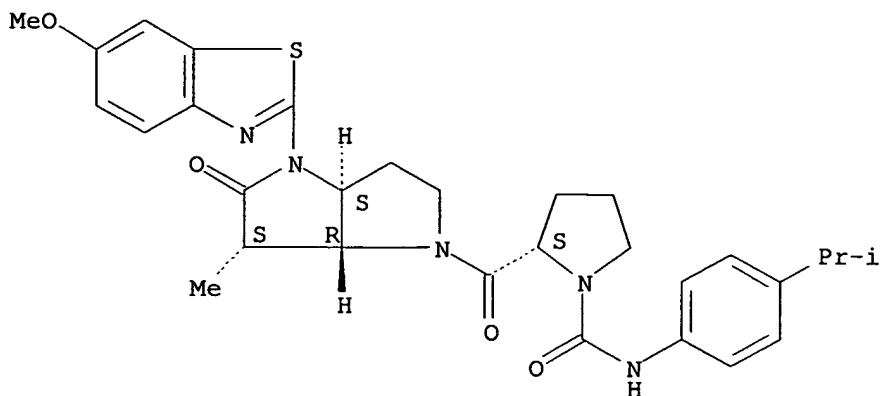
Absolute stereochemistry.



RN 214337-65-2 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-4-(6-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

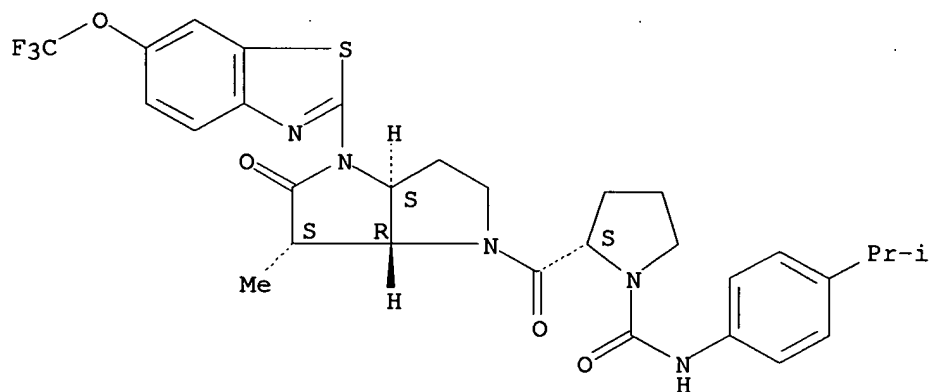
Absolute stereochemistry.



RN 214337-66-3 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-[6-(trifluoromethoxy)-2-benzothiazolyl]pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

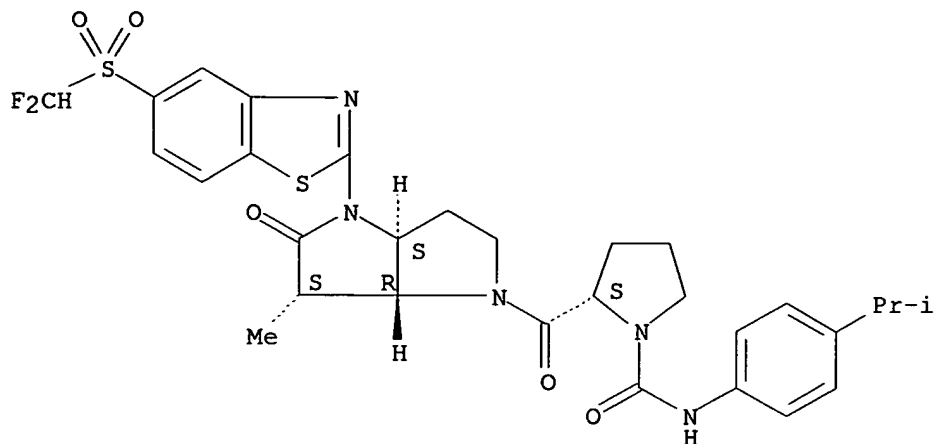
Absolute stereochemistry.



RN 214337-68-5 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-4-[5-[(difluoromethyl)sulfonyl]-2-benzothiazolyl]hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

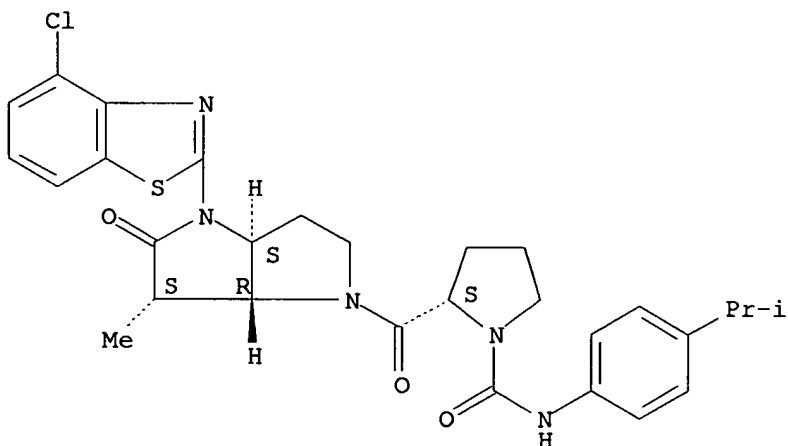
Absolute stereochemistry.



RN 628725-94-0 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-4-(4-chloro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

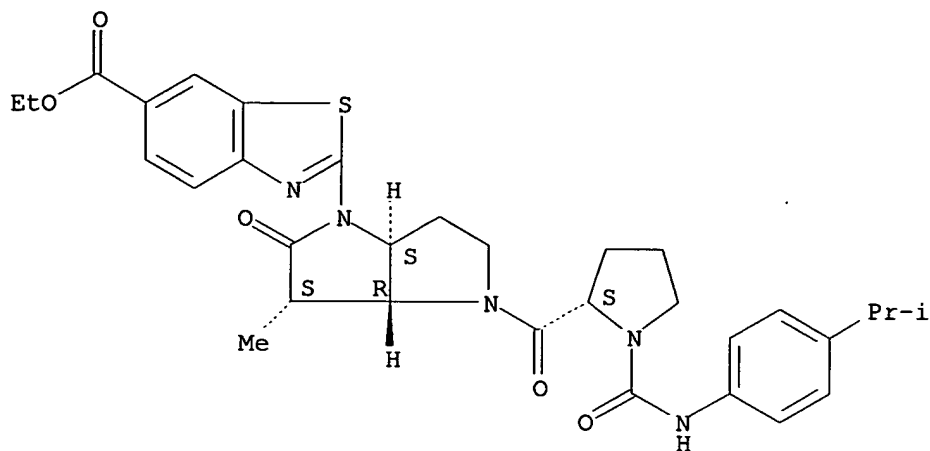
Absolute stereochemistry.



RN 628725-95-1 CAPLUS

CN 6-Benzothiazolecarboxylic acid, 2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[[[(2S)-1-[[[4-(1-methylethyl)phenyl]amino]carbonyl]-2-pyrrolidinyl]carbonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-, ethyl ester (9CI) (CA INDEX NAME)

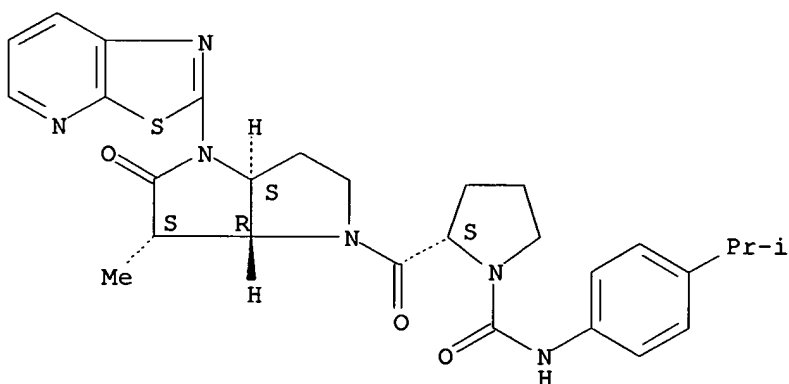
Absolute stereochemistry.



RN 628725-96-2 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-thiazolo[5,4-b]pyridin-2-yl]pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 214337-18-5P 214337-31-2P 214337-32-3P
 214337-33-4P 214337-37-8P 214337-41-4P
 214337-43-6P 214337-45-8P 214337-47-0P
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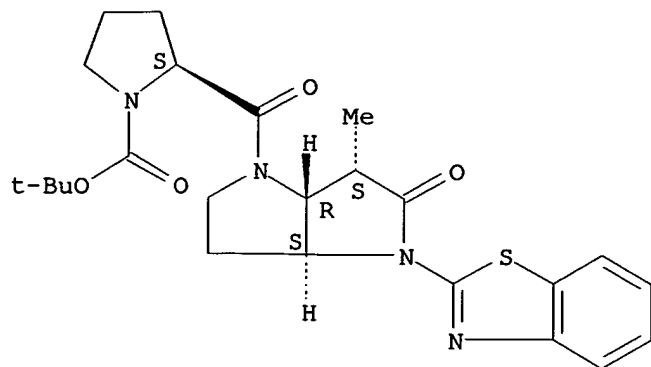
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and antiviral structure activity relationships of pyrrolidine-lactams as inhibitors of human cytomegalovirus protease)

RN 214337-18-5 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

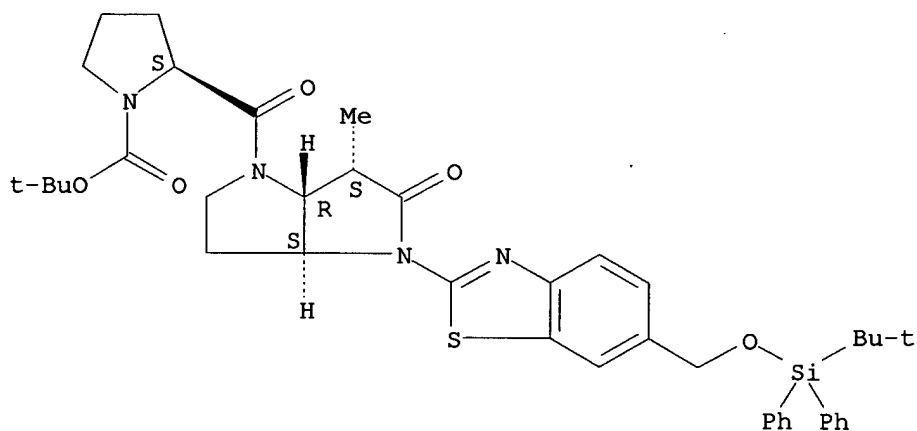
Absolute stereochemistry.



RN 214337-31-2 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-4-[6-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-benzothiazolyl]hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

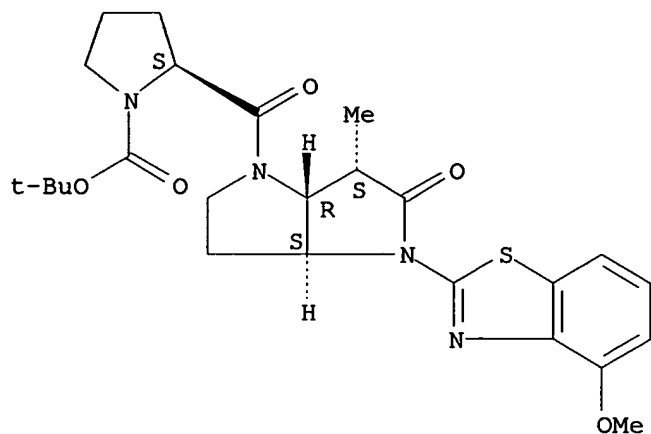
Absolute stereochemistry.



RN 214337-32-3 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-hexahydro-4-(4-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

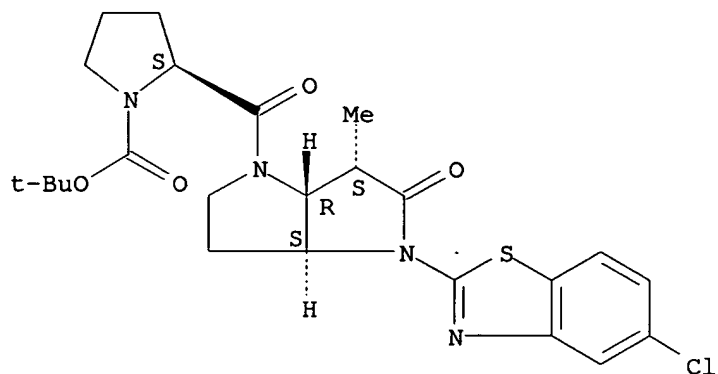
Absolute stereochemistry.



RN 214337-33-4 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-4-(5-chloro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

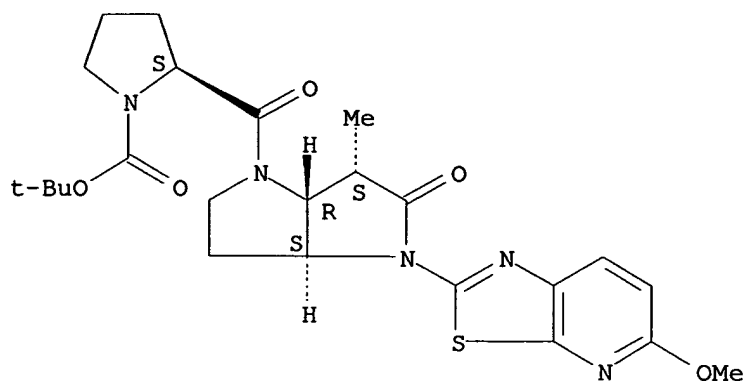
Absolute stereochemistry.



RN 214337-37-8 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-hexahydro-4-(5-methoxythiazolo[5,4-b]pyridin-2-yl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

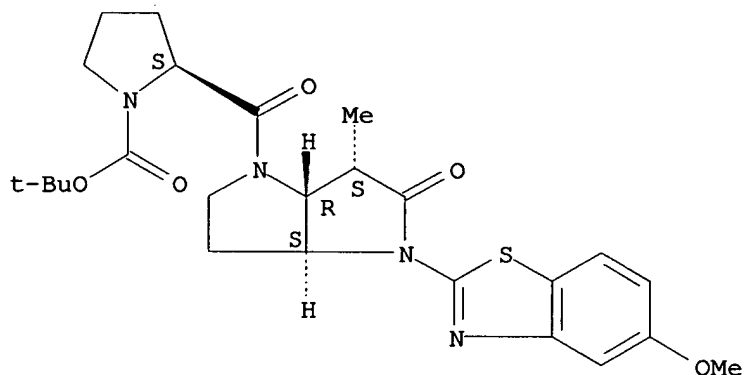
Absolute stereochemistry.



RN 214337-41-4 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-hexahydro-4-(5-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

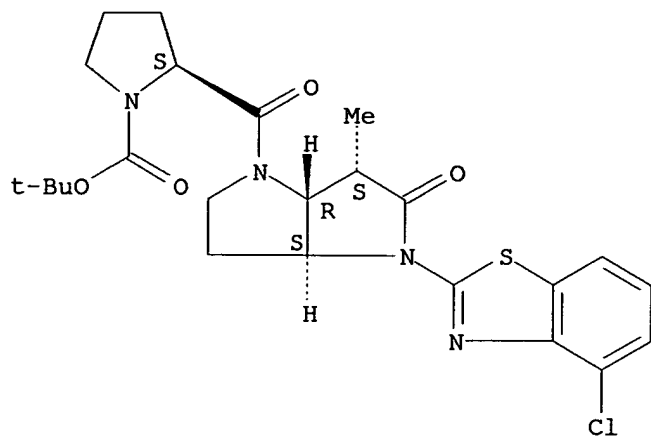
Absolute stereochemistry.



RN 214337-43-6 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-4-(4-chloro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

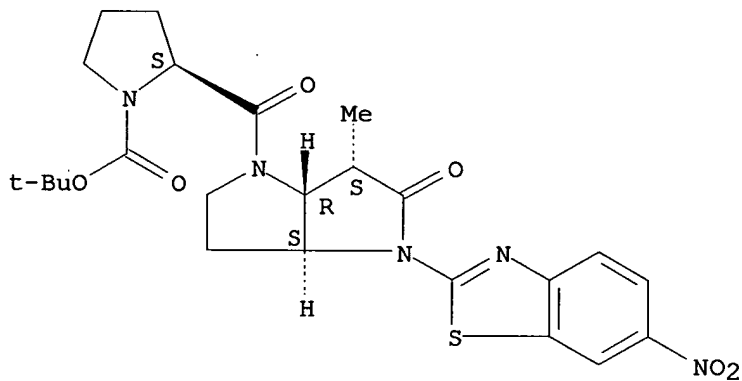
Absolute stereochemistry.



RN 214337-45-8 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-hexahydro-6-methyl-4-(6-nitro-2-benzothiazolyl)-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

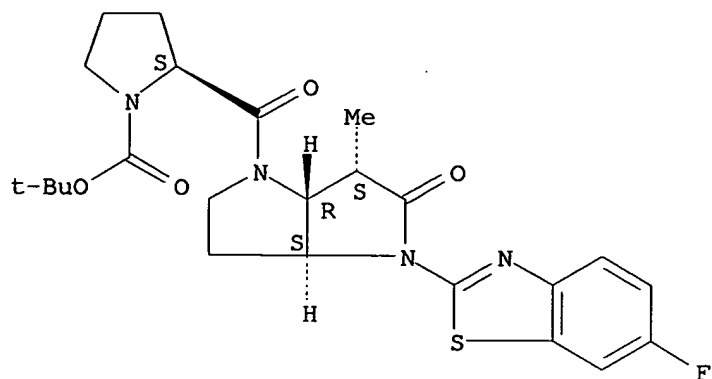
Absolute stereochemistry.



RN 214337-47-0 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-4-(6-fluoro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

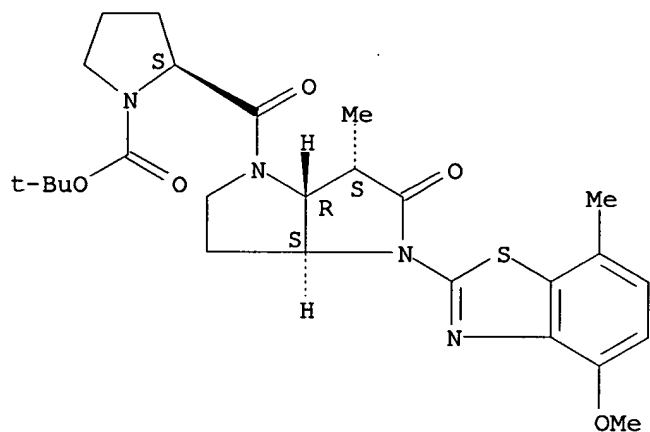
Absolute stereochemistry.



RN 214337-50-5 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-hexahydro-4-(4-methoxy-7-methyl-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

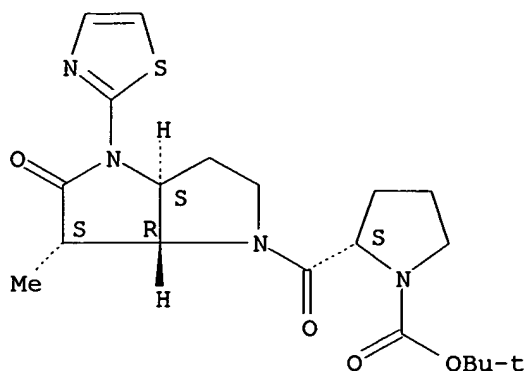
Absolute stereochemistry.



RN 214337-55-0 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-(2-thiazolyl)pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

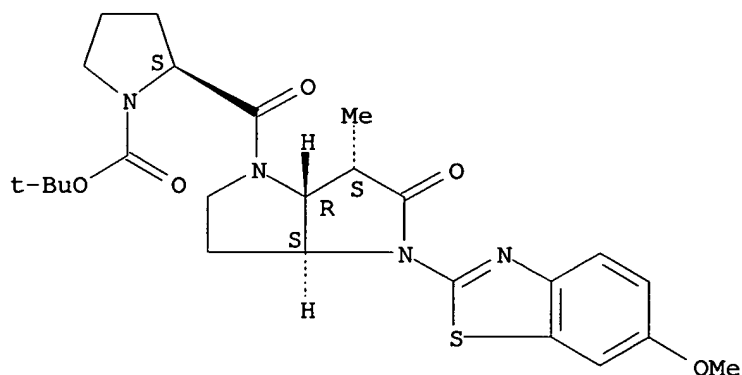
Absolute stereochemistry.



RN 628725-89-3 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-hexahydro-4-(6-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

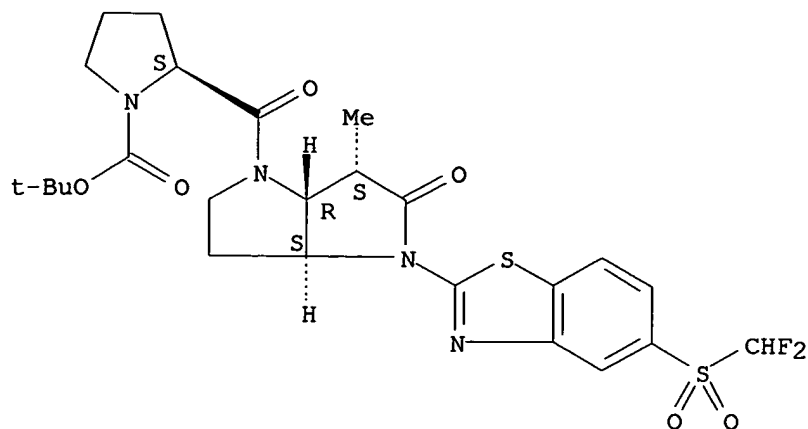
Absolute stereochemistry.



RN 628725-90-6 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-4-[5-[(difluoromethyl)sulfonyl]-2-benzothiazolyl]hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

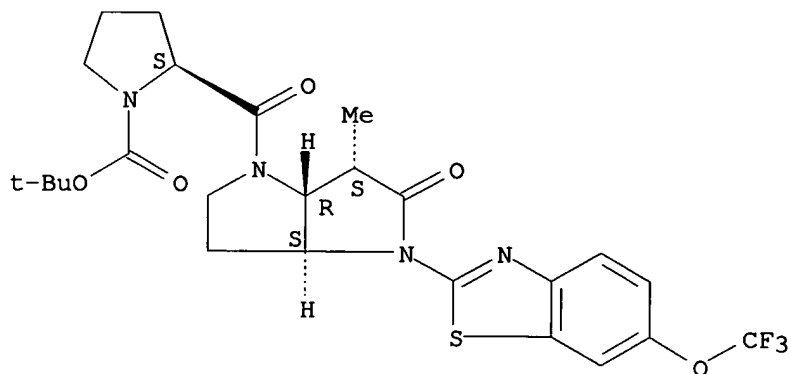
Absolute stereochemistry.



RN 628725-91-7 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-[6-(trifluoromethoxy)-2-benzothiazolyl]pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

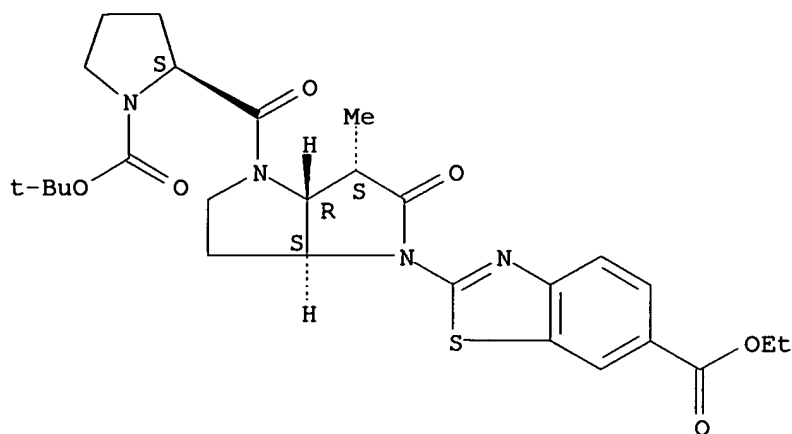
Absolute stereochemistry.



RN 628725-92-8 CAPLUS

CN 6-Benzothiazolecarboxylic acid, 2-[(3S,3aR,6aS)-4-[[[(2S)-1-[(1,1-dimethylethoxy)carbonyl]-2-pyrrolidinyl]carbonyl]hexahydro-3-methyl-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-, ethyl ester (9CI) (CA INDEX NAME)

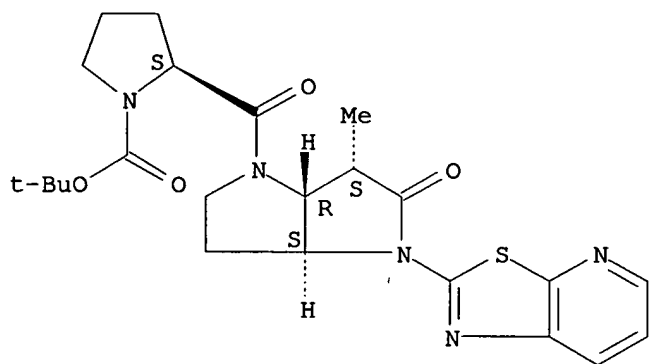
Absolute stereochemistry.



RN 628725-93-9 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-thiazolo[5,4-b]pyridin-2-ylpyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

20

THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~L10~~ ANSWER 11 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:438617 CAPLUS

DOCUMENT NUMBER: 138:100337

TITLE: Pyrrolidine-5,5-trans-lactams as novel mechanism-based inhibitors of human cytomegalovirus protease. Part 3: potency and plasma stability

AUTHOR(S): Borthwick, Alan D.; Exall, Anne M.; Haley, Terry M.; Jackson, Deborah L.; Mason, Andrew M.; Weingarten, Gordon G.

CORPORATE SOURCE: GlaxoSmithKline Research and Development, Department of Medicinal Chemistry CVU UK, Medicines Research Centre, Gunnels Wood Road, Herts, Stevenage, SG1 2NY, UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(13), 1719-1722

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:100337

AB Mechanism-based inhibitors of HCMV protease, which are stable to human plasma (≥ 20 h) and have single-figure potency in the μM range against HCMV protease, have been developed based on the dansylproline α -Me pyrrolidine-5,5-trans-lactam nucleus.

IT **214336-86-4P 486446-18-8P**

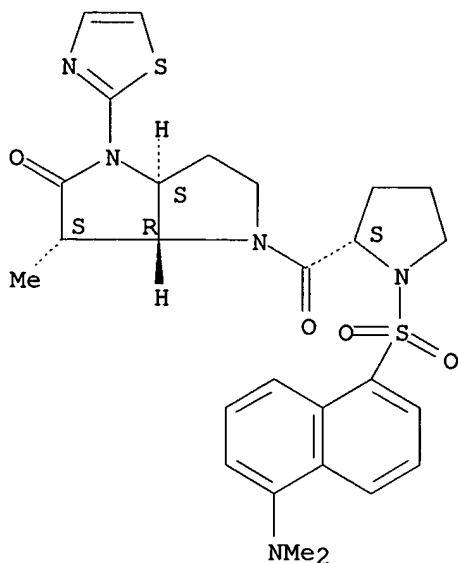
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(structure-activity relationship of pyrrolidine-5,5-trans-lactams as novel mechanism-based inhibitors of human cytomegalovirus protease)

RN 214336-86-4 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 4-[[[(2S)-1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-2-pyrrolidinyl]carbonyl]hexahydro-3-methyl-1-(2-thiazolyl)-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

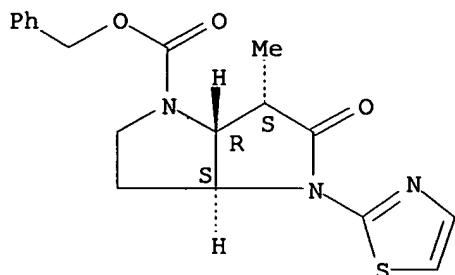


10/810,999

RN 486446-18-8 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-carboxylic acid, hexahydro-6-methyl-5-oxo-4-(2-thiazolyl)-, phenylmethyl ester, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 486446-24-6P

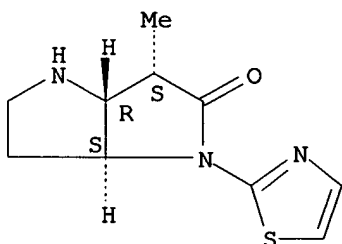
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(structure-activity relationship of pyrrolidine-5,5-trans-lactams as novel mechanism-based inhibitors of human cytomegalovirus protease)

RN 486446-24-6 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, hexahydro-3-methyl-1-(2-thiazolyl)-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 12 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:798225 CAPLUS

DOCUMENT NUMBER: 135:344471

TITLE: Preparation of diazabicyclic compounds as central nervous system active agents

INVENTOR(S): Schrimpf, Michael R.; Tietje, Karin R.; Toupence, Richard B.; Ji, Jianguo; Basha, Anwer; Bunnelle, William H.; Daanen, Jerome F.; Pace, Jennifer M.; Sippy, Kevin B.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 190 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

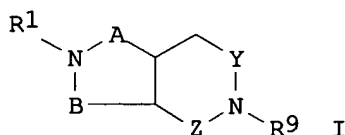
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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WO 2001081347	A2	20011101	WO 2001-US13798	20010427
WO 2001081347	A3	20020131		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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BR 2001007246	A	20021001	BR 2001-7246	20010427
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ZA 2002008274	A	20040211	ZA 2002-8274	20021014
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US 2004186107	A1	20040923	US 2004-810999	20040326
PRIORITY APPLN. INFO.:			US 2000-200111P	P 20000427
			US 2000-559943	A 20000427
			US 2001-833914	A 20010412
			WO 2001-US13798	W 20010427

OTHER SOURCE(S): MARPAT 135:344471

GI

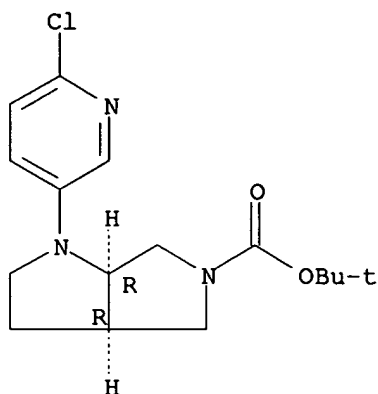


- AB Diazabicyclic compds. (I; e.g. cis-2-(3-pyridinyl)octahydropyrrolo[3,4-c]pyrrole dihydrochloride), pharmaceutical compns. of these compds., and use of said compns. to control synaptic transmission in mammals are claimed. In I: A = covalent bond, CH₂, CH₂CH₂, and CH₂CH₂CH₂; B = CH₂ and CH₂CH₂, provided that when A is CH₂CH₂CH₂, then B is CH₂; Y = covalent bond, CH₂, and CH₂CH₂; Z = covalent bond, CH₂, and CH₂CH₂, provided that when Y is CH₂CH₂, then Z is a covalent bond and further provided that when Z is CH₂CH₂, then Y is a covalent bond. R₁ = optionally substituted phthalazin-1-yl, pyridin-3-yl, pyrazinyl, pyrimidin-5-yl, pyridazin-3-yl, quinolin-3-yl, thieno[3,2-b]pyridin-2-yl, furano[3,2-b]pyridin-2-yl, thieno[3,2-b]pyridin-3-yl, furano[3,2-b]pyridin-3-yl, furano[3,2-b]pyridin-6-yl, thieno[3,2-b]pyridin-6-yl, furano[2,3-b]pyridin-5-yl, thieno[2,3-b]pyridin-5-yl, isothiazol-5-yl, isoxazol-5-yl. R₉ = H, alkoxycarbonyl, alkyl, amino, aminoalkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy, hydroxyalkyl, and phenoxycarbonyl. Values are reported for nicotinic acetylcholine receptor binding potencies and effectiveness of nicotinic acetylcholine receptor ligands as analgesic agents and in the formalin test for some of the claimed compds. Ninety-six example preps. are given but the methods of preparation are not claimed. The crystal and mol. structures of (3aS,6aS)-5-[(4-nitrophenyl)sulfonyl]-1-((1R)-1-phenylethyl)octahydropyrrolo[3,4-b]pyrrole and tert-Bu (3S,4S)-4-(hydroxymethyl)-3-[(1S)-1-phenylethylamino]-1-piperidinecarboxylate were determined by x-ray crystallog.
- IT **370880-19-6P**, tert-Butyl cis-1-(6-chloro-3-pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-5(1H)-carboxylate
370880-20-9P, cis-1-(6-Chloro-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole **370880-24-3P**, (1R,5R)-6-Benzyl-2-(3-pyridinyl)-2,6-diazabicyclo[3.2.0]heptane **370882-36-3P**, (3AR,6aR)-1-(6-chloro-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole **370882-40-9P**, tert-Butyl (3aR,6aR)-1-(6-chloro-3-pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-5-(1H)-carboxylate **370882-45-4P**, (3AR,6aR)-1-(3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole **370882-47-6P**, tert-Butyl (3aR,6aR)-1-(3-pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-5(1H)-carboxylate **370882-52-3P**, (3AS,6aS)-1-(6-chloro-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole **370882-56-7P**, tert-Butyl (3aS,6aS)-1-(6-chloro-3-pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-5(1H)-carboxylate **370882-58-9P**, tert-Butyl (3aS,6aS)-1-(3-pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-5(1H)-carboxylate **370882-59-0P**, (3AS,6aS)-1-(3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole **370882-70-5P**, tert-Butyl (3aR,6aR)-1-(5-cyano-3-pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-5(1H)-carboxylate **370882-72-7P**, tert-Butyl (3aS,6aS)-1-[5-(benzyloxy)-3-pyridinyl]hexahydropyrrolo[3,4-b]pyrrole-5(1H)-carboxylate **370882-73-8P**, tert-Butyl (3aS,6aS)-1-(5-hydroxy-3-pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-5(1H)-carboxylate **370882-74-9P**, (3AS,6aS)-1-(5-hydroxy-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole **370882-75-0P**, 5-[(3AS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]nicotinonitrile **370882-77-2P**, tert-Butyl (3aS,6aS)-1-(5-cyano-3-pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-5(1H)-carboxylate
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of diazabicyclic compds. as central nervous system active agents)
- RN 370880-19-6 CAPLUS
- CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, 1-(6-chloro-3-

10/810,999

pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)-rel- (9CI) (CA INDEX NAME)

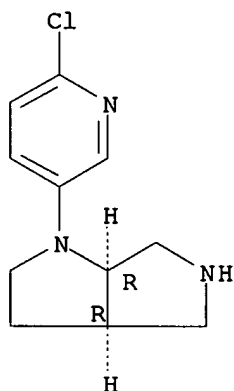
Relative stereochemistry.



RN 370880-20-9 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 1-(6-chloro-3-pyridinyl)octahydro-, (3aR,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

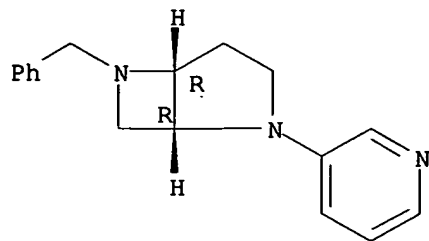


23a

RN 370880-24-3 CAPLUS

CN 2,6-Diazabicyclo[3.2.0]heptane, 6-(phenylmethyl)-2-(3-pyridinyl)-, (1R,5R)- (9CI) (CA INDEX NAME)

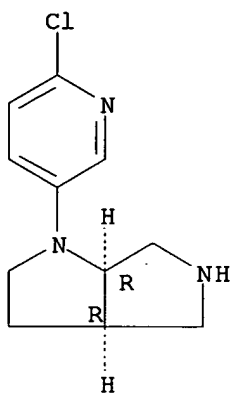
Absolute stereochemistry.



RN 370882-36-3 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 1-(6-chloro-3-pyridinyl)octahydro-, (3aR,6aR)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

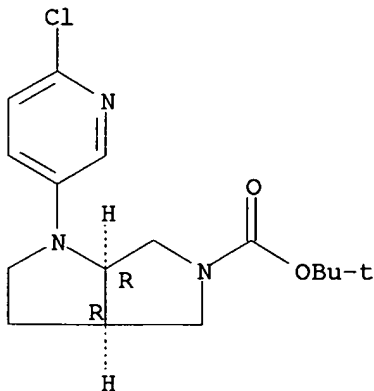


23c

RN 370882-40-9 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, 1-(6-chloro-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

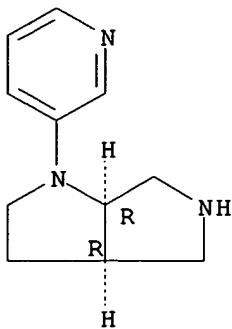


RN 370882-45-4 CAPLUS

10/810,999

CN Pyrrolo[3,4-b]pyrrole, octahydro-1-(3-pyridinyl)-, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

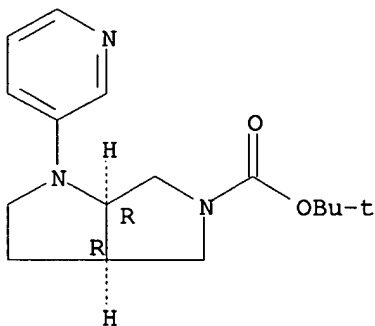


23d

RN 370882-47-6 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, hexahydro-1-(3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

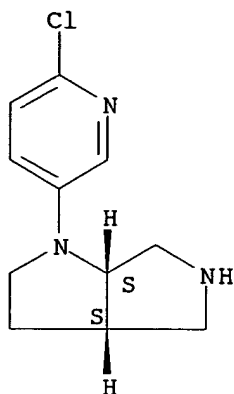


RN 370882-52-3 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 1-(6-chloro-3-pyridinyl)octahydro-, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

2,

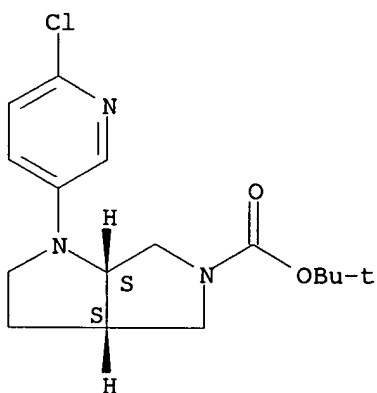


23e

RN 370882-56-7 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, 1-(6-chloro-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX NAME)

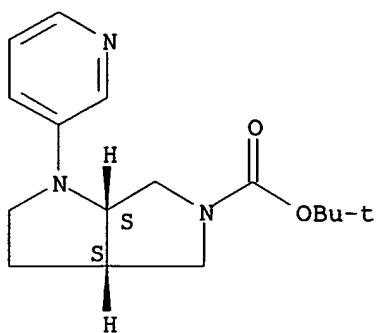
Absolute stereochemistry.



RN 370882-58-9 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, hexahydro-1-(3-pyridinyl)-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX NAME)

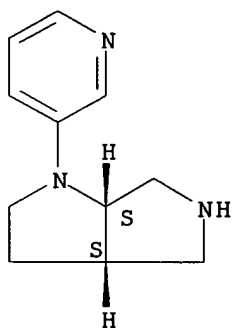
Absolute stereochemistry.



RN 370882-59-0 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, octahydro-1-(3-pyridinyl)-, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

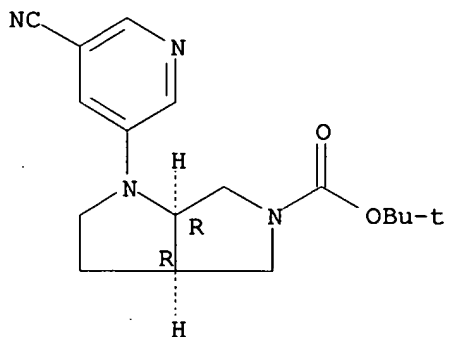


238

RN 370882-70-5 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, 1-(5-cyano-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



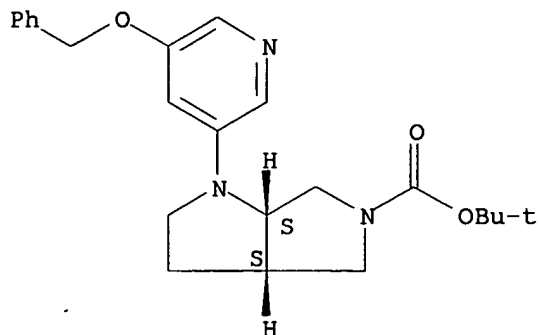
RN 370882-72-7 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, hexahydro-1-[5-

10/810,999

(phenylmethoxy)-3-pyridinyl]-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI)
(CA INDEX NAME)

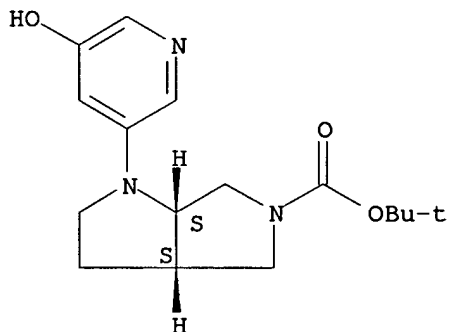
Absolute stereochemistry.



RN 370882-73-8 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, hexahydro-1-(5-hydroxy-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX NAME)

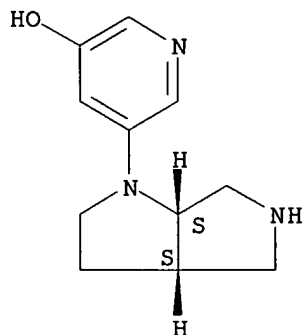
Absolute stereochemistry.



RN 370882-74-9 CAPLUS

CN 3-Pyridinol, 5-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

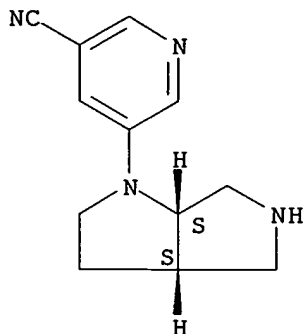


23h

RN 370882-75-0 CAPLUS

CN 3-Pyridinecarbonitrile, 5-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

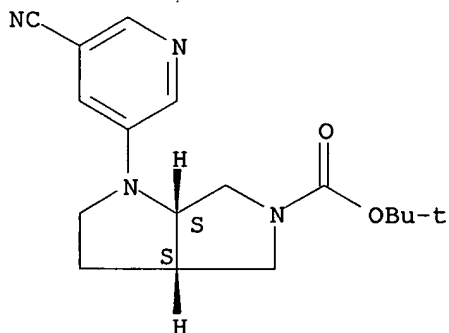


236

RN 370882-77-2 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-5(1H)-carboxylic acid, 1-(5-cyano-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



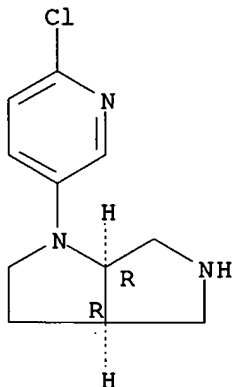
IT **370880-18-5P**, cis-1-(6-Chloro-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole monohydrochloride **370880-21-0P**, cis-1-(6-Chloro-3-pyridinyl)-5-methyloctahydropyrrolo[3,4-b]pyrrole monohydrochloride **370880-22-1P**, (1R,5R)-2-(3-Pyridinyl)-2,6-diazabicyclo[3.2.0]heptane **370880-23-2P**, (1R,5R)-2-(3-Pyridinyl)-2,6-diazabicyclo[3.2.0]heptane bis(4-methylbenzenesulfonate) **370882-37-4P**, (3AR,6AR)-1-(6-chloro-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole monofumarate **370882-46-5P**, (3AR,6AR)-1-(3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole monofumarate **370882-53-4P**, (3AS,6AS)-1-(6-chloro-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole monofumarate **370882-57-8P**, (3AS,6AS)-1-(3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole dihydrochloride **370882-69-2P**, 5-[(3AR,6AR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]nicotinonitrile fumarate (10:13) **370882-71-6P**, (3AS,6AS)-1-(5-hydroxy-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole dihydrochloride **370882-76-1P**, 5-[(3AS,6AS)-hexahydropyrrolo[3,4-

b]pyrrol-1(2H)-yl]nicotinonitrile monofumarate **370883-35-5P**,
 cis-1-(6-Chloro-3-pyridinyl)-5-methyloctahydropyrrolo[3,4-b]pyrrole
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of diazabicyclic compds. as central nervous system active
 agents)

RN 370880-18-5 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 1-(6-chloro-3-pyridinyl)octahydro-,
 monohydrochloride, (3aR,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

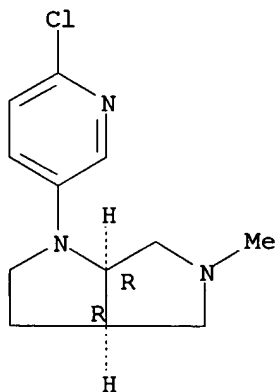


● HCl

RN 370880-21-0 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 1-(6-chloro-3-pyridinyl)octahydro-5-methyl-,
 monohydrochloride, (3aR,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



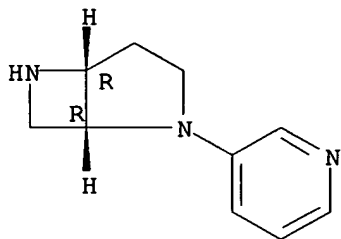
● HCl

10/810,999

RN 370880-22-1 CAPLUS

CN 2,6-Diazabicyclo[3.2.0]heptane, 2-(3-pyridinyl)-, (1R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 370880-23-2 CAPLUS

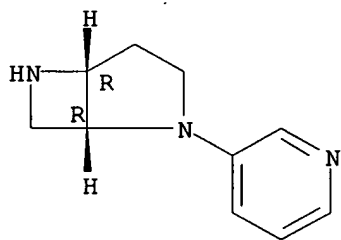
CN 2,6-Diazabicyclo[3.2.0]heptane, 2-(3-pyridinyl)-, (1R,5R)-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 370880-22-1

CMF C10 H13 N3

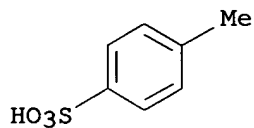
Absolute stereochemistry.



CM 2

CRN 104-15-4

CMF C7 H8 O3 S



RN 370882-37-4 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 1-(6-chloro-3-pyridinyl)octahydro-, (3aR,6aR)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

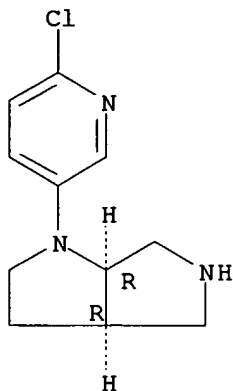
10/810,999

CM 1

CRN 370882-36-3

CMF C11 H14 Cl N3

Absolute stereochemistry.

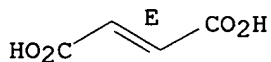


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RN 370882-46-5 CAPLUS

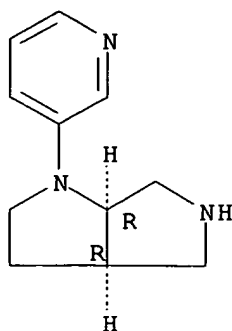
CN Pyrrolo[3,4-b]pyrrole, octahydro-1-(3-pyridinyl)-, (3aR,6aR)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-45-4

CMF C11 H15 N3

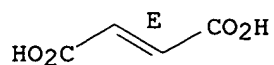
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

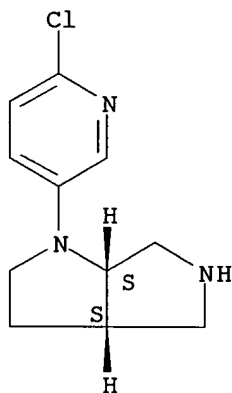


RN 370882-53-4 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 1-(6-chloro-3-pyridinyl)octahydro-, (3aS,6aS)-,
(2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-52-3
CMF C11 H14 Cl N3

Absolute stereochemistry.



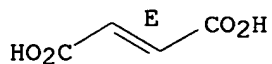
CM 2

CRN 110-17-8

10/810,999

CMF C4 H4 O4

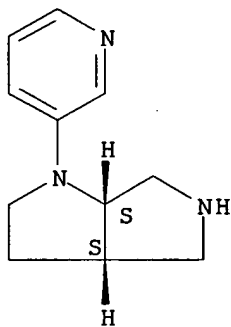
Double bond geometry as shown.



RN 370882-57-8 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, octahydro-1-(3-pyridinyl)-, dihydrochloride, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

RN 370882-69-2 CAPLUS

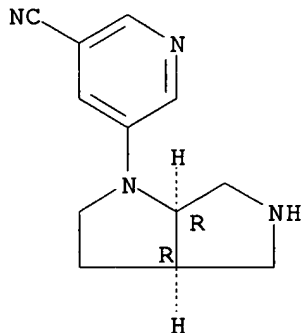
CN 3-Pyridinecarbonitrile, 5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-, (2E)-2-butenedioate (10:13) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-68-1

CMF C12 H14 N4

Absolute stereochemistry.



23 g)

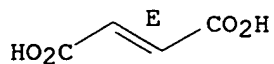
10/810,999

CM 2

CRN 110-17-8

CMF C4 H4 O4

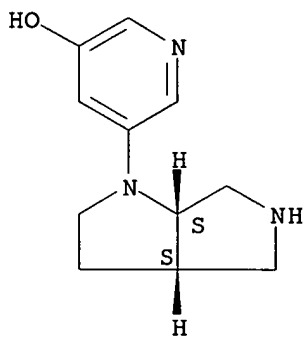
Double bond geometry as shown.



RN 370882-71-6 CAPLUS

CN 3-Pyridinol, 5-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

RN 370882-76-1 CAPLUS

CN 3-Pyridinecarbonitrile, 5-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

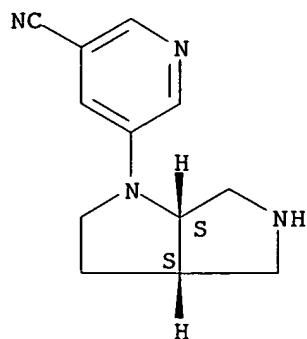
CM 1

CRN 370882-75-0

CMF C12 H14 N4

Absolute stereochemistry.

10/810,999

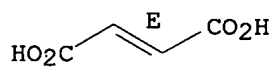


CM 2

CRN 110-17-8

CMF C4 H4 O4

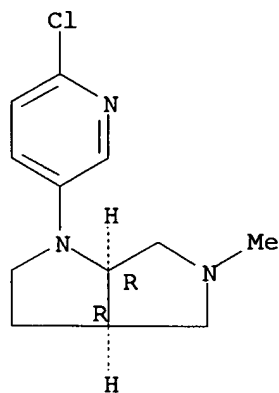
Double bond geometry as shown.



RN 370883-35-5 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 1-(6-chloro-3-pyridinyl)octahydro-5-methyl-,
(3aR,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



23b

10/810,999

~~110~~ ANSWER 13 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:573269 CAPLUS

DOCUMENT NUMBER: 135:152805

TITLE: Preparation of benzimidazoles as ORL1-receptor agonists for analgesics

INVENTOR(S): Ito, Fumitaka; Noguchi, Hirohide; Ohashi, Yoriko; Shimokawa, Hirohisa

PATENT ASSIGNEE(S): Pfizer Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 39 pp.

CODEN: JKXXAF

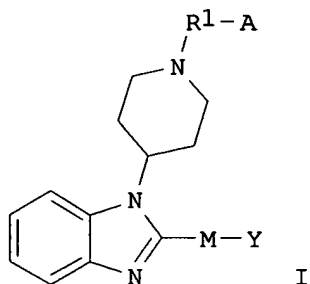
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001213878	A2	20010807	JP 2000-396414	20001227
JP 3392402	B2	20030331		
EP 1122257	A1	20010808	EP 2000-311316	20001218
EP 1122257	B1	20051012		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 306488	E	20051015	AT 2000-311316	20001218
CA 2330092	AA	20010705	CA 2001-2330092	20010103
CA 2330092	C	20050322		
US 2002049212	A1	20020425	US 2001-753954	20010103
US 6861425	B2	20050301		
BR 2001000014	A	20010828	BR 2001-14	20010104
PRIORITY APPLN. INFO.:			US 2000-174542P	P 20000105
OTHER SOURCE(S):	MARPAT	135:152805		
GI				



AB Title compds. I [R1 = C3-11 cycloalkyl, C6-16 bicycloalkyl, C6-16 tricycloalkyl, C8-16 tetracycloalkyl, etc.; A = (un)substituted C1-7 alkyl, C2-5 alkenyl, C2-5 alkynyl, aryl, etc.; M = single bond, CH2, O, S, SO, SO2, CO, NH, etc.; Y = 4- to 12-membered bicyclic carbon ring, 4- to 12-membered bicyclic hetero ring, 5- to 17-membered spiro carbon ring, 5- to 17-membered spiro hetero ring; Z1-Z4 = (un)substituted C1-4 alkyl, C1-4 alkoxy, C1-4 alkylsulfonyl, C1-4 alkylcarbonyl, carboxy, etc.] or their salts are prepared Tert-Bu 3-[1-[1-(1-phenylcycloheptyl)-4-piperidinyl]-1H-benzimidazol-2-yl]-3,8-diazabicyclo[3.2.1]octane-8-carboxylate was treated

with F3CCO₂H in CH₂Cl₂ at room temperature for 0.5 h to give 77.6%
2-(3,8-diazabicyclo[3.2.1]oct-3-yl)-1-[1-(1-phenylcycloheptyl)-4-
piperidinyl]-1H-benzimidazole HCl salt.

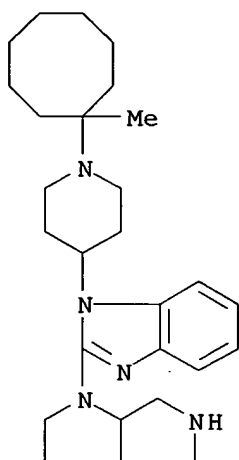
IT 352542-26-8P 352542-27-9P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzimidazoles as ORL1-receptor agonists for analgesics)

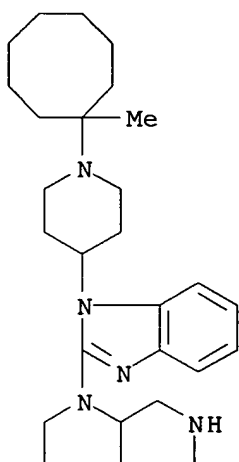
RN 352542-26-8 CAPLUS

CN 1H-Benzimidazole, 2-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)-1-[1-(1-methylcyclooctyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)



RN 352542-27-9 CAPLUS

CN 1H-Benzimidazole, 2-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)-1-[1-(1-methylcyclooctyl)-4-piperidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

~~L10~~ ANSWER 14 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:842126 CAPLUS

DOCUMENT NUMBER: 134:17404

TITLE: Preparation of heterocyclic substituted aminoazacycles
useful as central nervous system agents

INVENTOR(S): Schrimpf, Michael R.; Sippy, Kevin B.; Daanen, Jerome
F.; Ryther, Keith B.; Ji, Jianguo

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

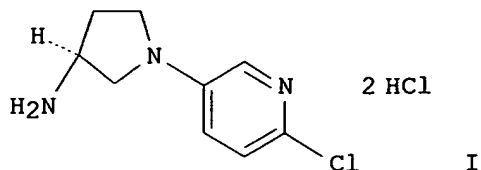
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000071534	A1	20001130	WO 2000-US13339	20000515
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6833370	B1	20041221	US 2000-559881	20000426
CA 2373793	AA	20001130	CA 2000-2373793	20000515
EP 1178982	A1	20020213	EP 2000-932445	20000515
EP 1178982	B1	20040630		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000007229	A	20020910	BR 2000-7229	20000515
JP 2003500402	T2	20030107	JP 2000-619791	20000515
NZ 515207	A	20030926	NZ 2000-515207	20000515
EP 1428824	A1	20040616	EP 2004-5194	20000515
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AT 270288	E	20040715	AT 2000-932445	20000515
PT 1178982	T	20041130	PT 2000-932445	20000515
ES 2226844	T3	20050401	ES 2000-932445	20000515
AU 781241	B2	20050512	AU 2000-50166	20000515
CN 1636990	A	20050713	CN 2004-10085561	20000515
ZA 2001009162	A	20030206	ZA 2001-9162	20011106
NO 2001005669	A	20011123	NO 2001-5669	20011120
BG 106192	A	20020830	BG 2001-106192	20011207
HK 1045305	A1	20050401	HK 2002-105306	20020717
US 2005043291	A1	20050224	US 2004-946669	20040922
PRIORITY APPLN. INFO.:			US 1999-316707	A 19990521
			US 2000-559881	A 20000426
			US 1999-135372P	P 19990521
			EP 2000-932445	A3 20000515
			WO 2000-US13339	W 20000515

OTHER SOURCE(S): MARPAT 134:17404
GI



AB Title compds. [Z-R3, wherein Z is a defined aminoazacycle and R3 is a defined heterocycle moiety] and pharmaceutically acceptable salts are prepared and pharmaceutical compns. of these compds., useful in controlling synaptic transmission in mammals, are claimed. Thus, the title compound I was prepared and tested, in vivo and in vitro, as nicotinic acetylcholine receptor.

IT **309962-77-4P**

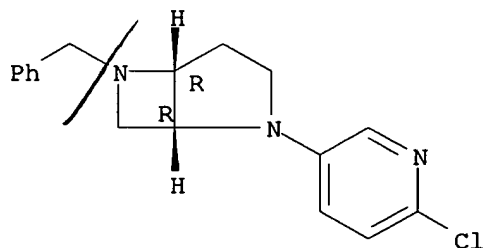
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocyclic substituted aminoazacycles useful as central nervous system agents)

RN 309962-77-4 CAPLUS

CN 2,6-Diazabicyclo[3.2.0]heptane, 2-(6-chloro-3-pyridinyl)-6-(phenylmethyl)-, (1R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/810,999

110 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:227661 CAPLUS

DOCUMENT NUMBER: 132:265186

TITLE: Preparation of pyrrolopyrrolone derivatives as antiviral agents

INVENTOR(S): Borthwick, Alan David; Davies, David Evan; Exall, Anne Marjorie; Leahy, John Henry; Rahim, George Saad; Shah, Pritom; Sollis, Stephen; Weingarten, Gordon Gad

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 175 pp.

CODEN: PIXXD2

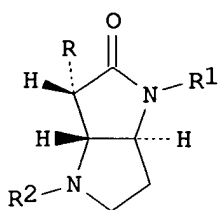
DOCUMENT TYPE: Patent

LANGUAGE: English

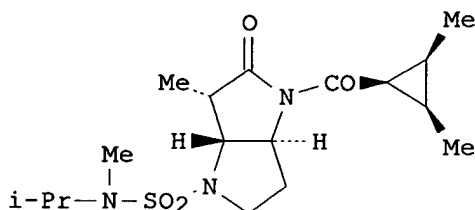
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000018770	A1	20000406	WO 1999-GB3244	19990930
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 9961084	A1	20000417	AU 1999-61084	19990930
PRIORITY APPLN. INFO.:			GB 1998-21199	A 19980930
			WO 1999-GB3244	W 19990930
OTHER SOURCE(S):	MARPAT 132:265186			
GI				



I



II

AB The title bicyclic compds. (I) [wherein R = H or (un)substituted alkyl; R1 = (un)substituted (fused) heteroaryl with 1-4 heteroatoms, or acyl; R2 = SO2R3; R3 = alkyl, alkenyl, (un)substituted 3- to 7-membered N-heterocycle containing ≤ 2 heteroatoms, (un)substituted amino, etc.] were prepared for the treatment and prophylaxis of viral infections. I are particularly aimed at infections caused by viruses which encode for a serine protease enzyme, especially viruses of the Herpes family. Examples include syntheses for nearly 200 target compds. and their intermediates and data from 9 bioassays. For instance, (3aS,6S,6aR)-N-isopropyl-N,6-dimethyl-5-oxohexahydropyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide (preparation given) in THF was coupled with (cis, cis)-2,3-dimethylcyclopropylcarboxylic acid

anhydride in the presence of Li hexamethyldisilazide to give II (83%). II inhibited Herpes simplex virus 1 (HSV1) protease by 105% at 0.5 μM , displayed an IC_{50} of 0.98 μM against human cytomegalovirus (HCMV), and proved nontoxic in Vero cells at active concns. (CCID_{50} = 315 μM).

IT 214337-13-0P 214337-16-3P 263168-99-6P
 263169-00-2P 263169-03-5P 263169-05-7P
 263169-06-8P 263169-07-9P 263169-08-0P
 263169-09-1P 263169-10-4P 263169-11-5P
 263169-19-3P 263169-26-2P 263169-27-3P
 263169-30-8P 263169-31-9P

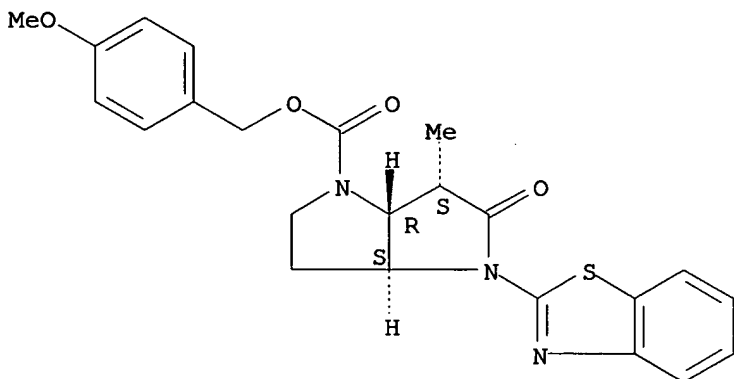
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; Preparation of pyrrolopyrrolone derivs. as antiviral agents)

RN 214337-13-0 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-carboxylic acid, 4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxo-, (4-methoxyphenyl)methyl ester, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 214337-16-3 CAPLUS

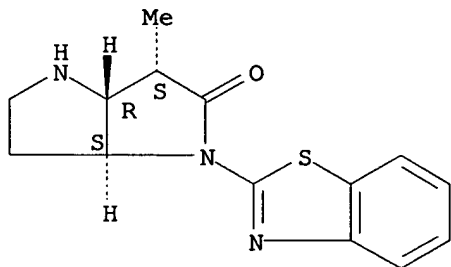
CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)hexahydro-3-methyl-, (3S,3aR,6aS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 214337-15-2

CMF C14 H15 N3 O S

Absolute stereochemistry.

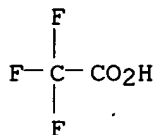


10/810,999

CM 2

CRN 76-05-1

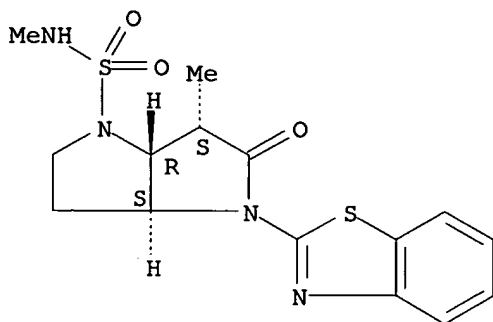
CMF C2 H F3 O2



RN 263168-99-6 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-N,6-dimethyl-5-oxo-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

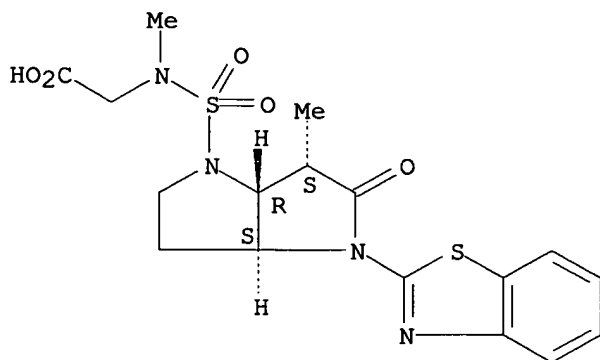
Absolute stereochemistry.



RN 263169-00-2 CAPLUS

CN Glycine, N-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

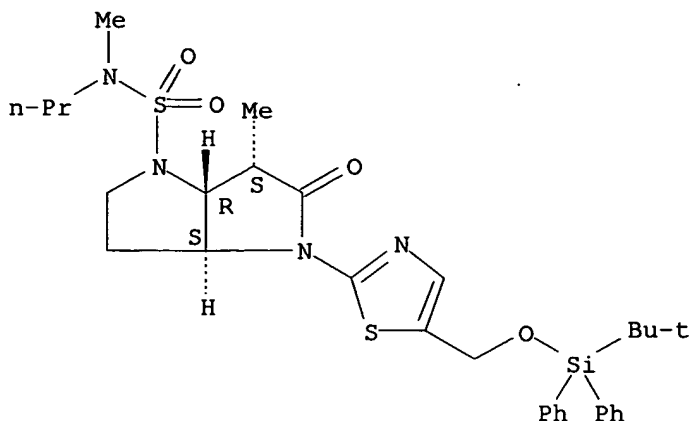


RN 263169-03-5 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[5-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-thiazolyl]hexahydro-N,6-dimethyl-

5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

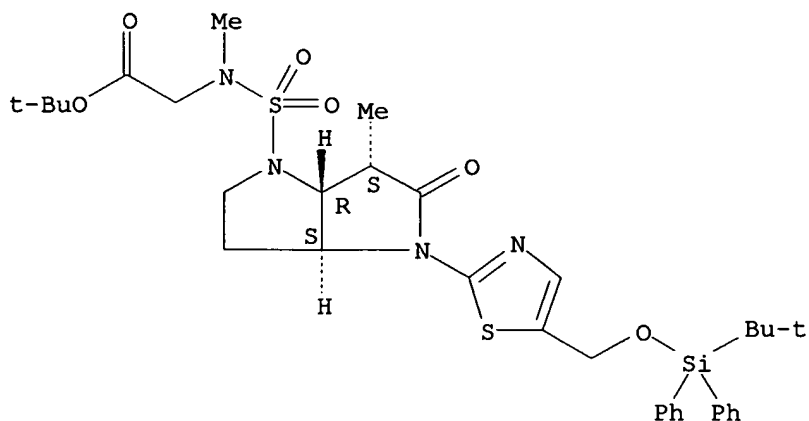
Absolute stereochemistry.



RN 263169-05-7 CAPLUS

CN Glycine, N-[[[(3aS,6S,6aR)-4-[5-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-thiazolyl]hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]-N-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

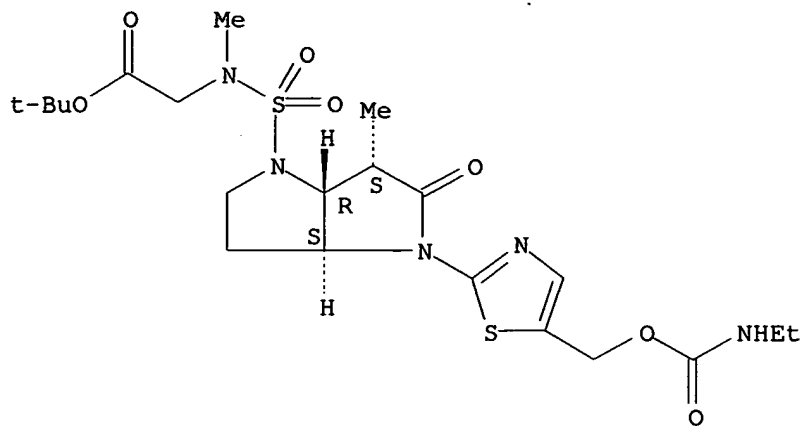
Absolute stereochemistry.



RN 263169-06-8 CAPLUS

CN Glycine, N-[[[(3aS,6S,6aR)-4-[5-[[[(ethylamino)carbonyl]oxy]methyl]-2-thiazolyl]hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]-N-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

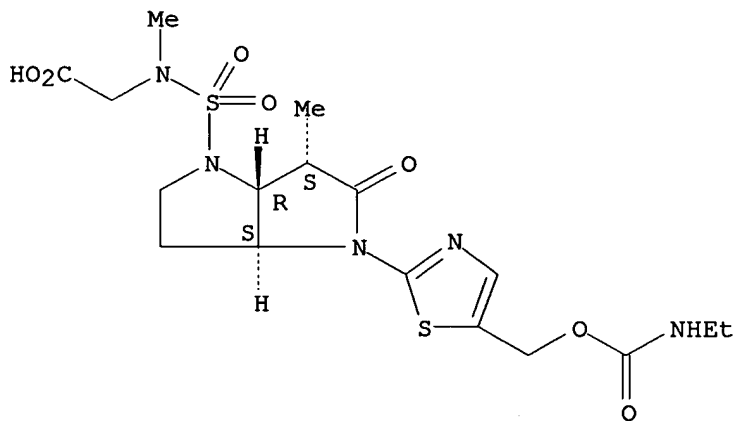
Absolute stereochemistry.



RN 263169-07-9 CAPLUS

CN Glycine, N-[[(3aS,6S,6aR)-4-[5-[[[(ethylamino) carbonyl]oxy]methyl]-2-thiazolyl]hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]-N-methyl- (9CI) (CA INDEX NAME)

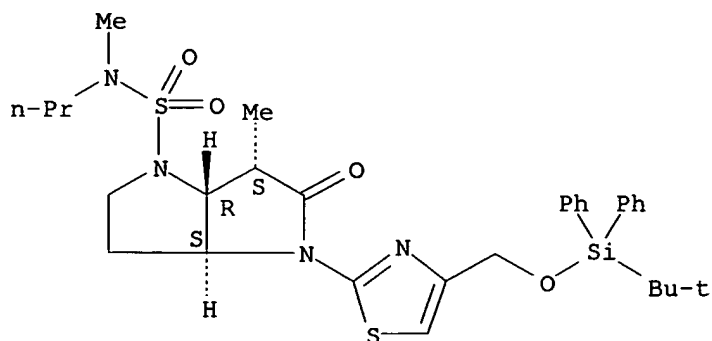
Absolute stereochemistry.



RN 263169-08-0 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[4-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-thiazolyl]hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

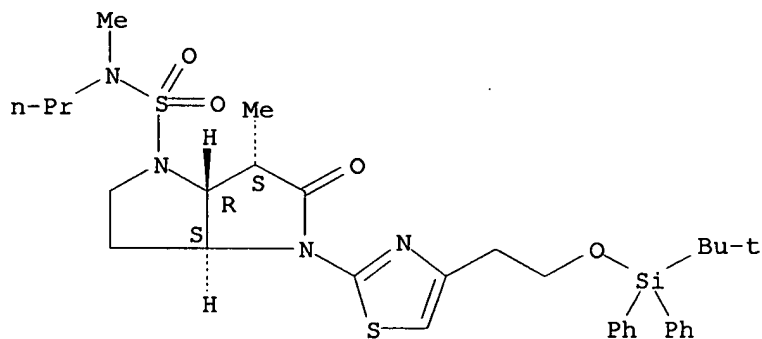
Absolute stereochemistry.



RN 263169-09-1 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[4-[2-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]ethyl]-2-thiazolyl]hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

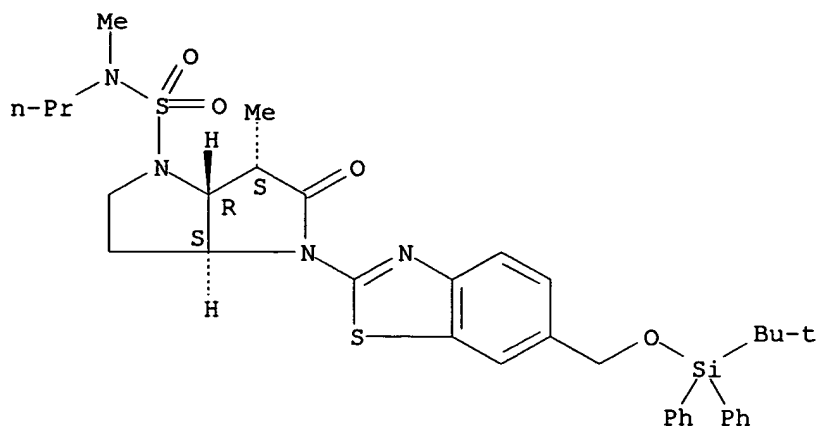
Absolute stereochemistry.



RN 263169-10-4 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[6-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-benzothiazolyl]hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

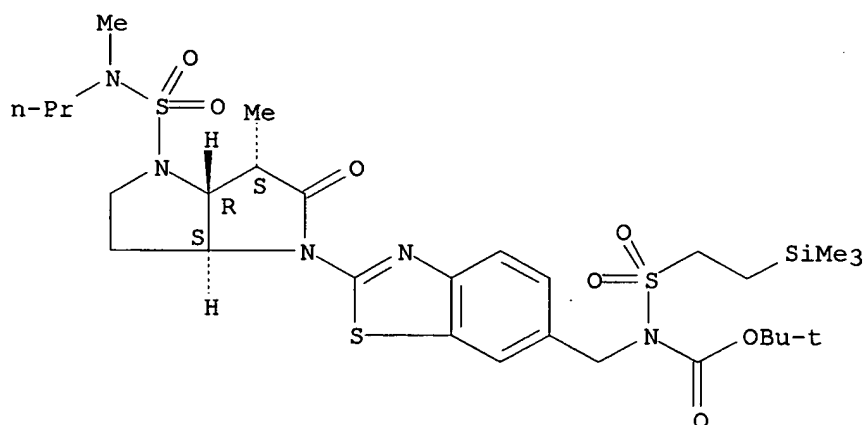
Absolute stereochemistry.



RN 263169-11-5 CAPLUS

CN Carbamic acid, [[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-6-benzothiazolyl]methyl][[2-(trimethylsilyl)ethyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

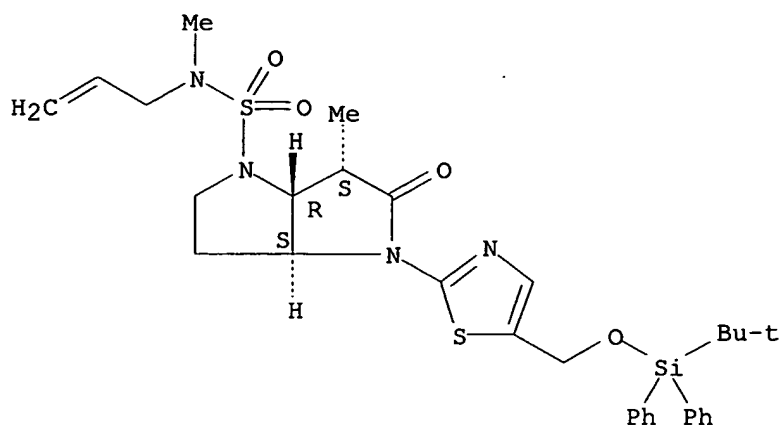
Absolute stereochemistry.



RN 263169-19-3 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[5-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-thiazolyl]hexahydro-N,6-dimethyl-5-oxo-N-2-propenyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

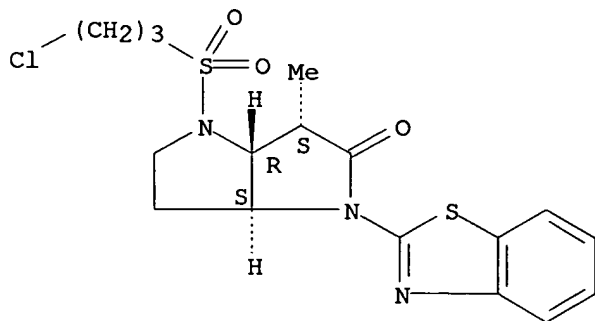
Absolute stereochemistry.



RN 263169-26-2 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)-4-[(3-chloropropyl)sulfonyl]hexahydro-3-methyl-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

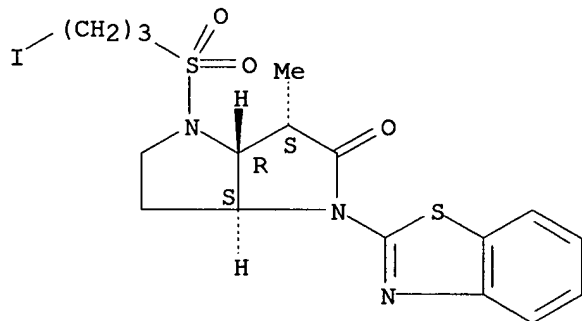
Absolute stereochemistry.



RN 263169-27-3 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)hexahydro-4-[(3-iodopropyl)sulfonyl]-3-methyl-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

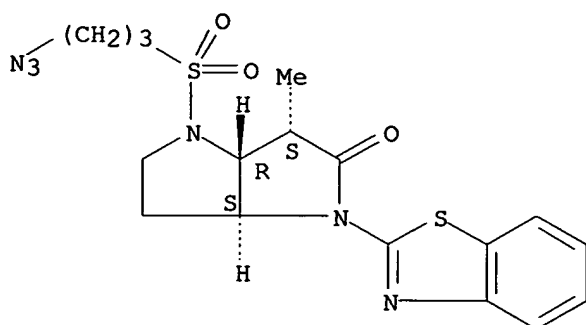


RN 263169-30-8 CAPLUS

10/810,999

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 4-[(3-azidopropyl)sulfonyl]-1-(2-benzothiazolyl)hexahydro-3-methyl-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

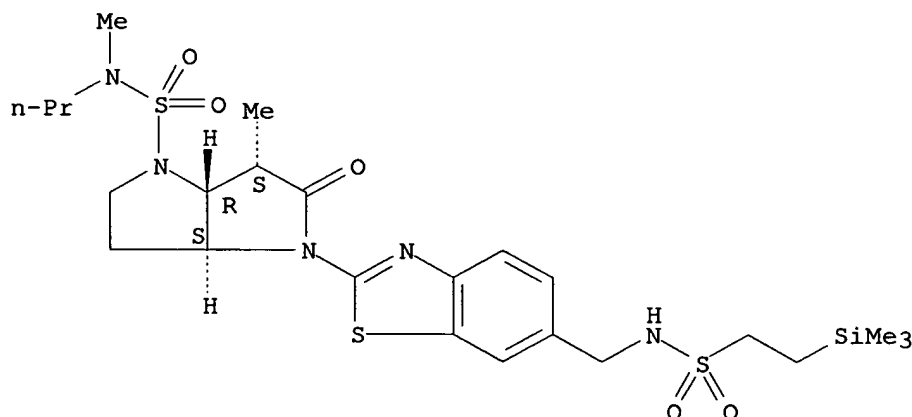
Absolute stereochemistry.



RN 263169-31-9 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-N,6-dimethyl-5-oxo-N-propyl-4-[6-[[[2-(trimethylsilyl)ethyl]sulfonyl]amino]methyl]-2-benzothiazolyl]-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 263167-20-0P 263167-30-2P 263167-84-6P
263167-85-7P 263167-86-8P 263167-87-9P
263167-94-8P 263167-97-1P 263168-01-0P
263168-10-1P 263168-12-3P 263168-13-4P
263168-14-5P 263168-84-9P

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

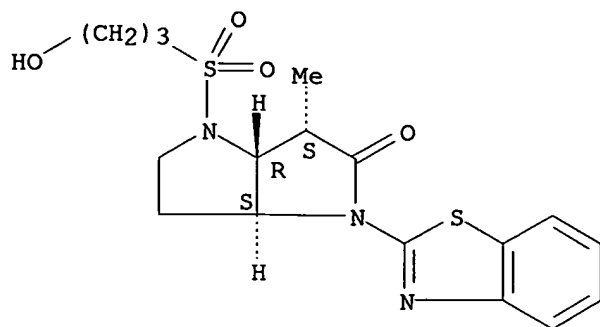
(target compound; Preparation of pyrrolopyrrolone derivs. as antiviral agents)

RN 263167-20-0 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)hexahydro-4-[(3-hydroxypropyl)sulfonyl]-3-methyl-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

10/810,999

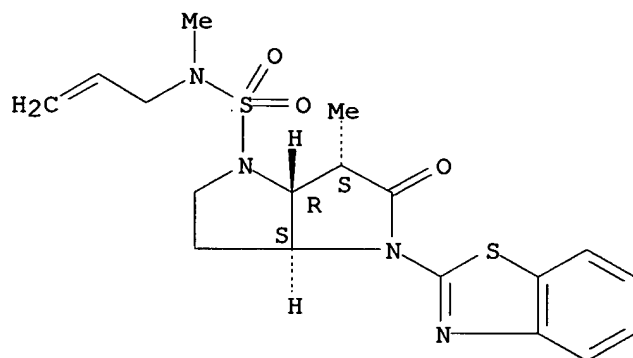
Absolute stereochemistry.



RN 263167-30-2 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-N,6-dimethyl-5-oxo-N-2-propenyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

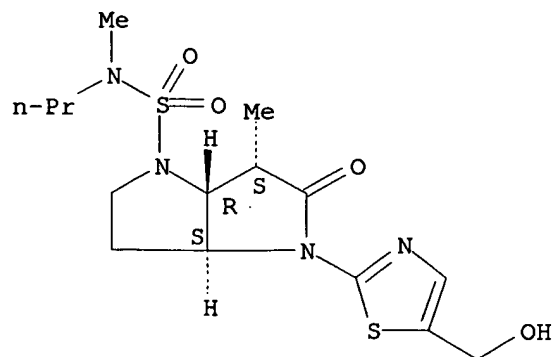
Absolute stereochemistry.



RN 263167-84-6 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-4-[5-(hydroxymethyl)-2-thiazolyl]-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

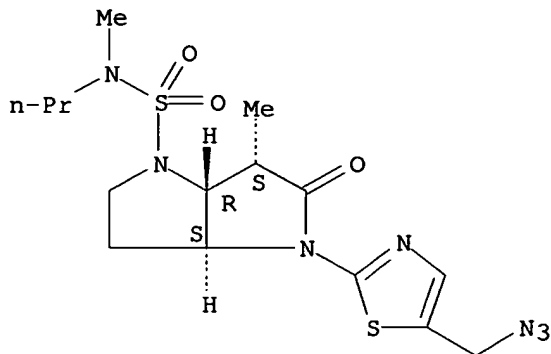


10/810,999

RN 263167-85-7 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[5-(azidomethyl)-2-thiazolyl]hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

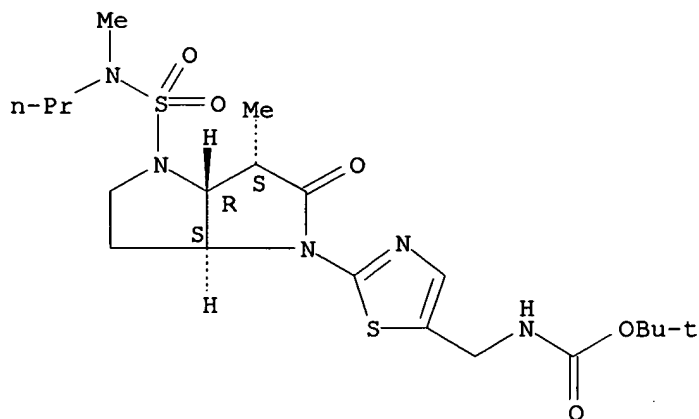
Absolute stereochemistry.



RN 263167-86-8 CAPLUS

CN Carbamic acid, [[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

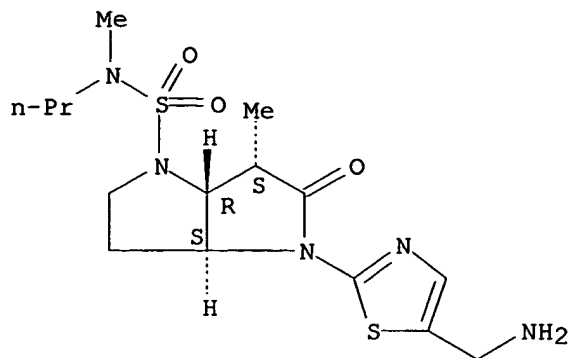
Absolute stereochemistry.



RN 263167-87-9 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[5-(aminomethyl)-2-thiazolyl]hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

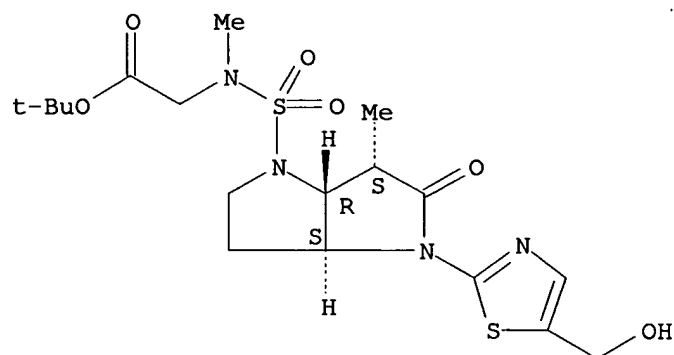
Absolute stereochemistry.



RN 263167-94-8 CAPLUS

CN Glycine, N-[[(3aS,6S,6aR)-hexahydro-4-[5-(hydroxymethyl)-2-thiazolyl]-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]-N-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

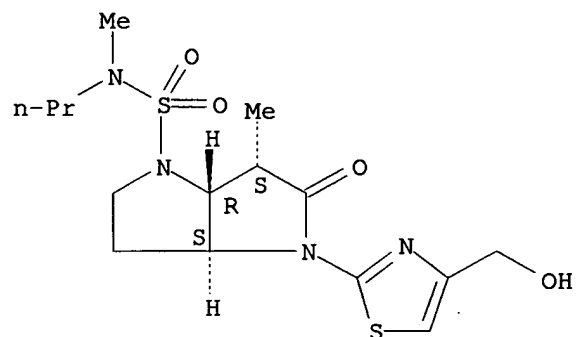
Absolute stereochemistry.



RN 263167-97-1 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-4-[4-(hydroxymethyl)-2-thiazolyl]-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

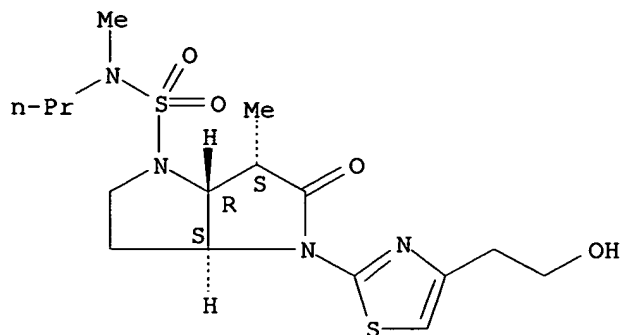
Absolute stereochemistry.



RN 263168-01-0 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-4-[4-(2-hydroxyethyl)-2-thiazolyl]-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)-(9CI) (CA INDEX NAME)

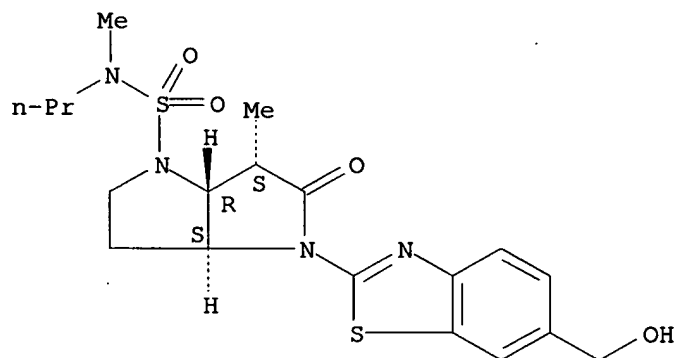
Absolute stereochemistry.



RN 263168-10-1 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-4-[6-(hydroxymethyl)-2-benzothiazolyl]-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)-(9CI) (CA INDEX NAME)

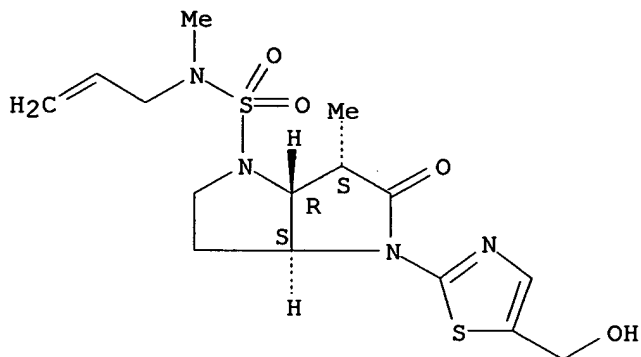
Absolute stereochemistry.



RN 263168-12-3 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-4-[5-(hydroxymethyl)-2-thiazolyl]-N,6-dimethyl-5-oxo-N-2-propenyl-, (3aS,6S,6aR)-(9CI) (CA INDEX NAME)

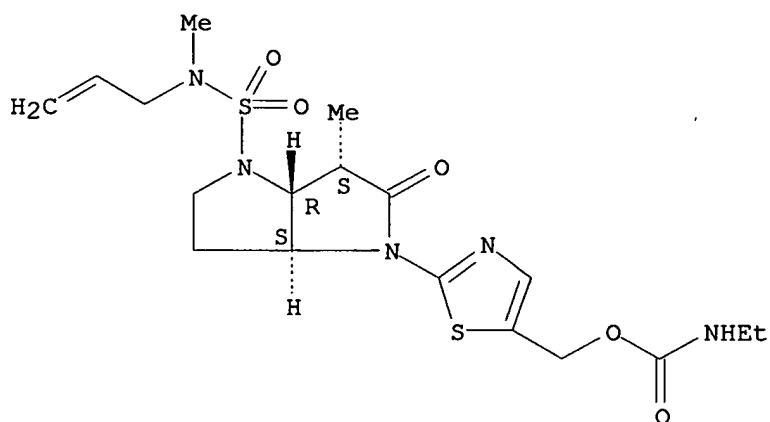
Absolute stereochemistry.



RN 263168-13-4 CAPLUS

CN Carbamic acid, ethyl-, [2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methyl-2-propenylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

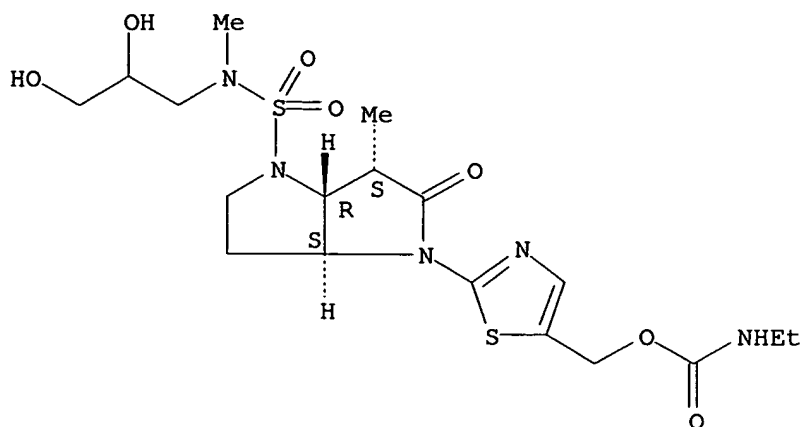
Absolute stereochemistry.



RN 263168-14-5 CAPLUS

CN Carbamic acid, ethyl-, [2-[(3S,3aR,6aS)-4-[[2,3-dihydroxypropyl)methylamino]sulfonyl]hexahydro-3-methyl-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

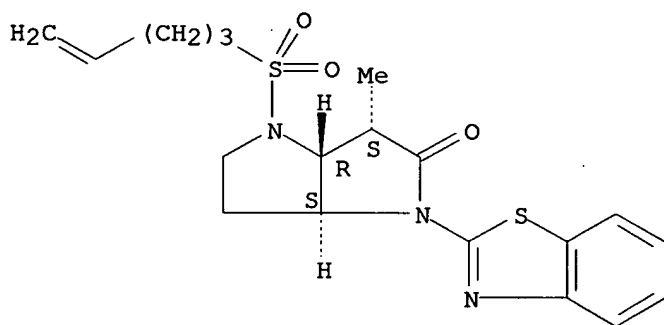
Absolute stereochemistry.



RN 263168-84-9 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)hexahydro-3-methyl-4-(4-pentenylsulfonyl)-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 263167-18-6P 263167-19-7P 263167-21-1P
 263167-22-2P 263167-23-3P 263167-24-4P
 263167-25-5P 263167-26-6P 263167-27-7P
 263167-28-8P 263167-29-9P 263167-31-3P
 263167-32-4P 263167-33-5P 263167-34-6P
 263167-35-7P 263167-37-9P 263167-38-0P
 263167-39-1P 263167-40-4P 263167-41-5P
 263167-42-6P 263167-43-7P 263167-44-8P
 263167-45-9P 263167-46-0P 263167-47-1P
 263167-48-2P 263167-49-3P 263167-50-6P
 263167-51-7P 263167-52-8P 263167-53-9P
 263167-54-0P 263167-55-1P 263167-56-2P
 263167-57-3P 263167-58-4P 263167-59-5P
 263167-60-8P 263167-61-9P 263167-62-0P
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 263167-66-4P 263167-67-5P 263167-68-6P
 263167-69-7P 263167-70-0P 263167-71-1P
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263167-96-0P 263167-98-2P 263167-99-3P
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 263168-83-8P 263168-85-0P 263168-86-1P
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 263169-66-0P 263169-67-1P

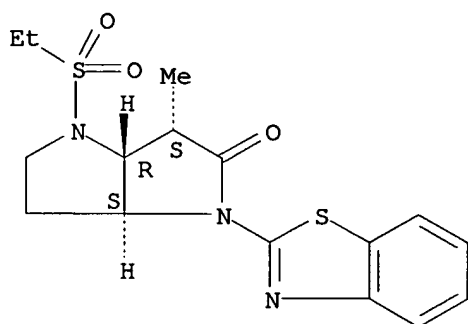
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; Preparation of pyrrolopyrrolone derivs. as antiviral agents)

RN 263167-18-6 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)-4-(ethylsulfonyl)hexahydro-3-methyl-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

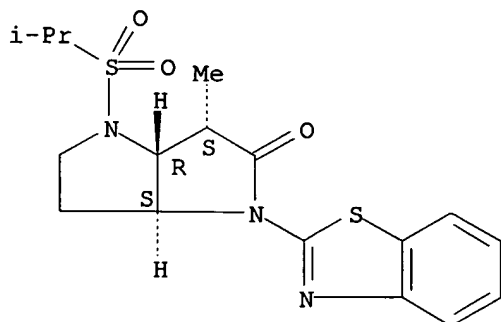
Absolute stereochemistry.



RN 263167-19-7 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)hexahydro-3-methyl-4-[(1-methylethyl)sulfonyl]-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

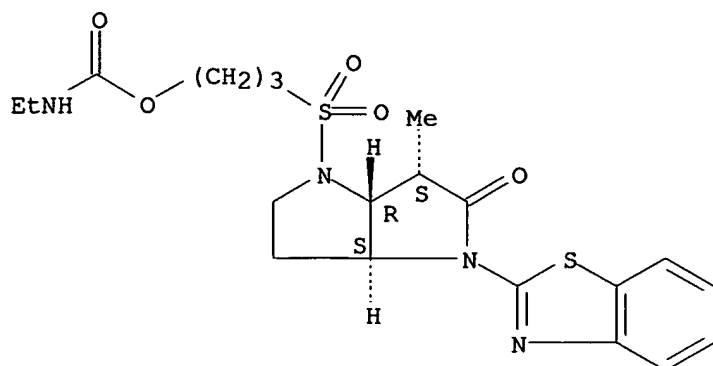
Absolute stereochemistry.



RN 263167-21-1 CAPLUS

CN Carbamic acid, ethyl-, 3-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]propyl ester (9CI) (CA INDEX NAME)

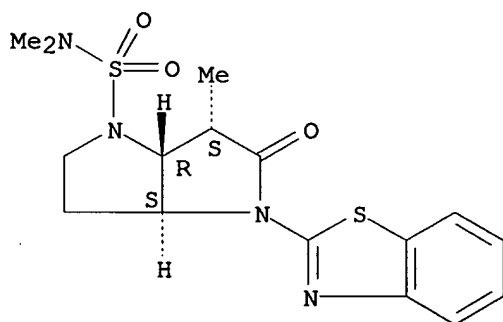
Absolute stereochemistry.



RN 263167-22-2 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-N,N,6-trimethyl-5-oxo-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

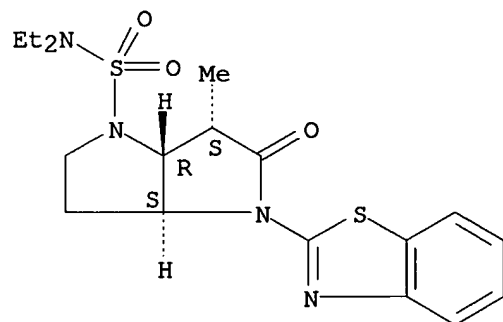
Absolute stereochemistry.



RN 263167-23-3 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)-N,N-diethylhexahydro-6-methyl-5-oxo-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

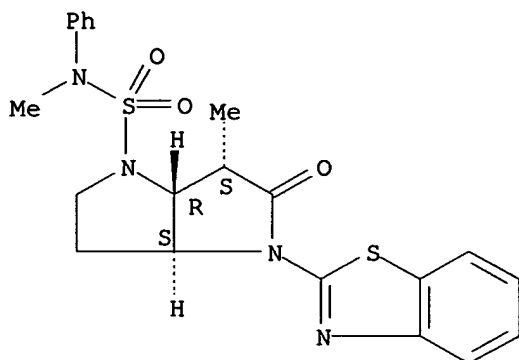
Absolute stereochemistry.



RN 263167-24-4 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-N,6-dimethyl-5-oxo-N-phenyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

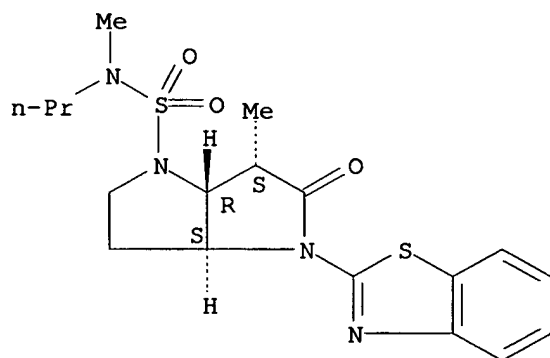
Absolute stereochemistry.



RN 263167-25-5 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

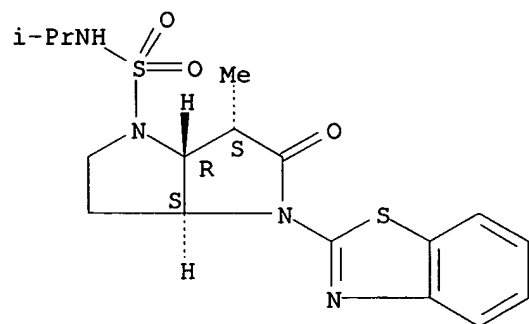
Absolute stereochemistry.



RN 263167-26-6 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-6-methyl-N-(1-methylethyl)-5-oxo-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

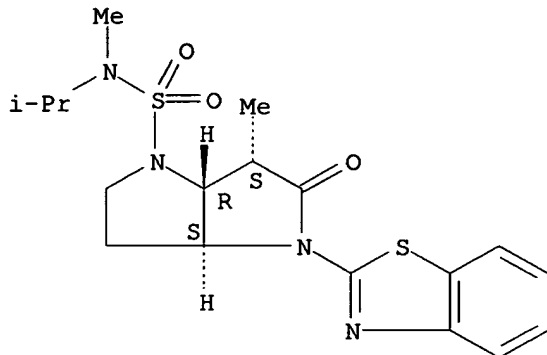


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RN 263167-27-7 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-N,6-dimethyl-N-(1-methylethyl)-5-oxo-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

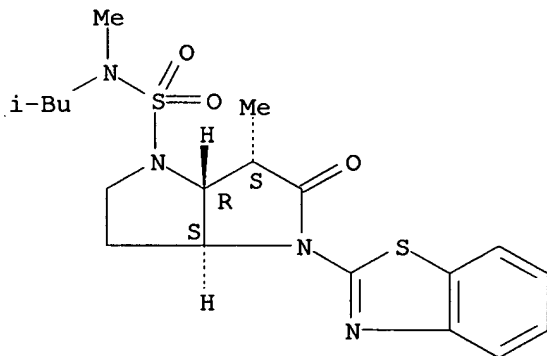
Absolute stereochemistry.



RN 263167-28-8 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-N,6-dimethyl-N-(2-methylpropyl)-5-oxo-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

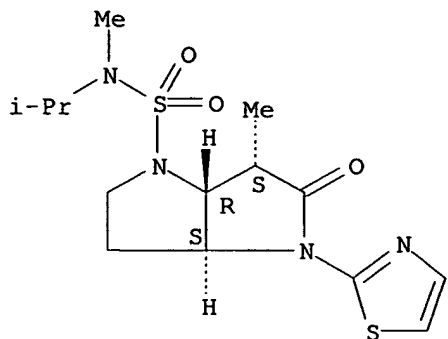
Absolute stereochemistry.



RN 263167-29-9 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-N,6-dimethyl-N-(1-methylethyl)-5-oxo-4-(2-thiazolyl)-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

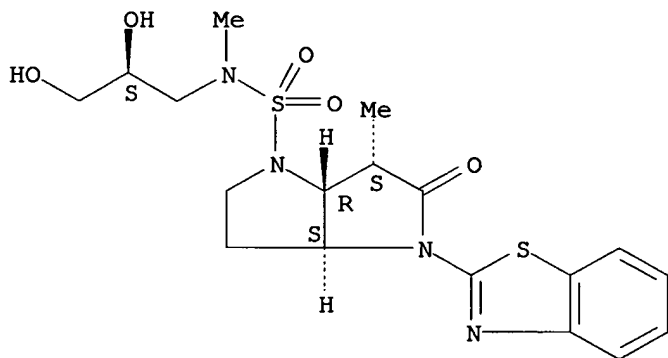
Absolute stereochemistry.



RN 263167-31-3 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)-N-[(2S)-2,3-dihydroxypropyl]hexahydro-N,6-dimethyl-5-oxo-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

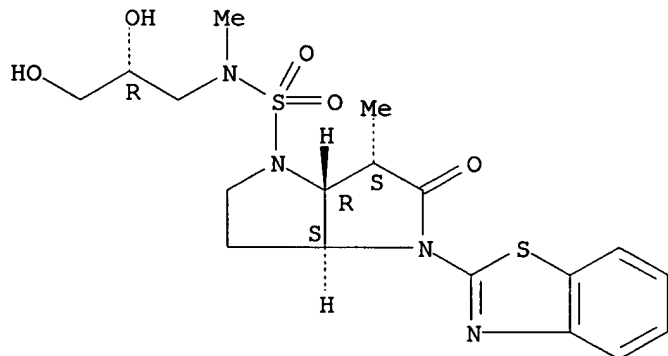
Absolute stereochemistry.



RN 263167-32-4 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)-N-[(2R)-2,3-dihydroxypropyl]hexahydro-N,6-dimethyl-5-oxo-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

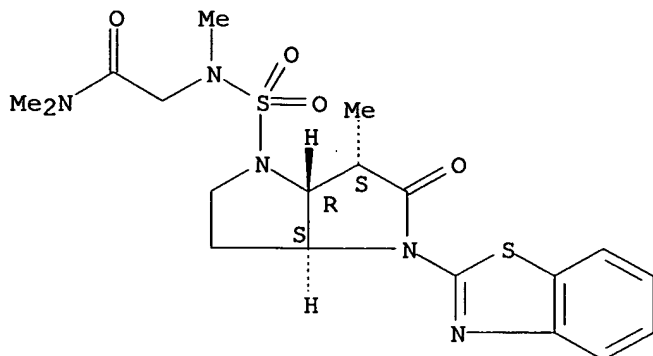
Absolute stereochemistry.



RN 263167-33-5 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N,N-dimethyl- (9CI)
(CA INDEX NAME)

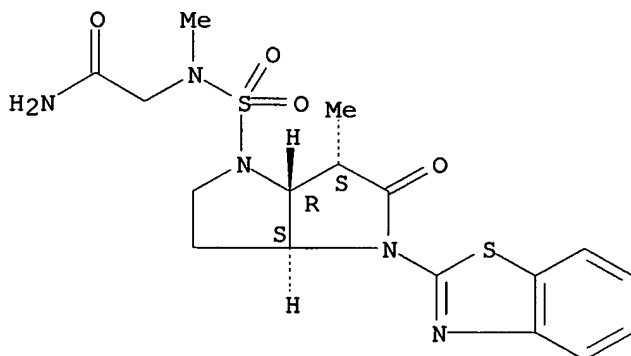
Absolute stereochemistry.



RN 263167-34-6 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]- (9CI) (CA INDEX NAME)

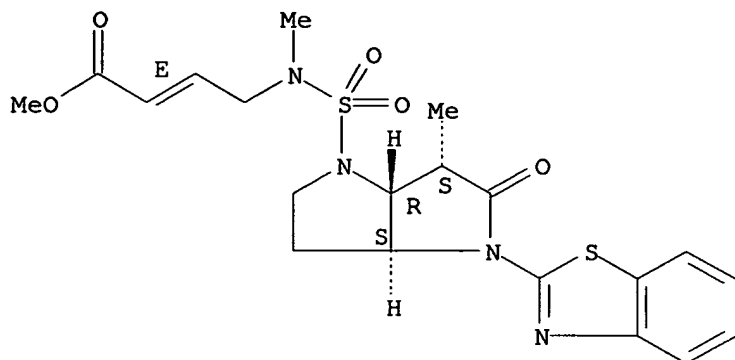
Absolute stereochemistry.



RN 263167-35-7 CAPLUS

CN 2-Butenoic acid, 4-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 263167-37-9 CAPLUS

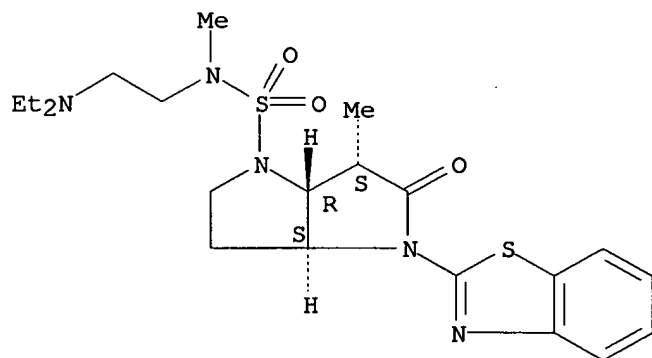
CN Formic acid, compd. with (3aS,6S,6aR)-4-(2-benzothiazolyl)-N-[2-(diethylamino)ethyl]hexahydro-N,6-dimethyl-5-oxopyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 263167-36-8

CMF C21 H31 N5 O3 S2

Absolute stereochemistry.



CM 2

CRN 64-18-6

CMF C H2 O2

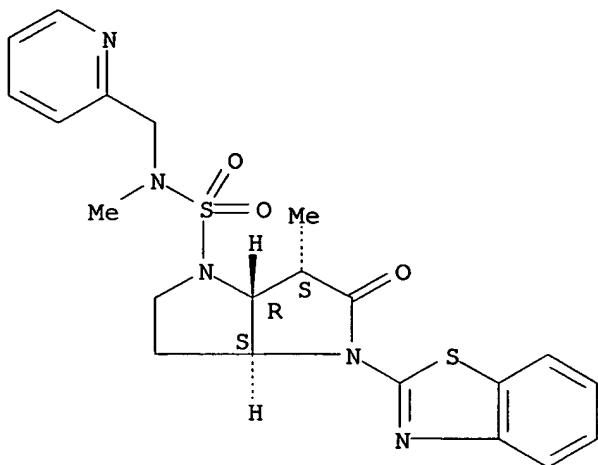
O=CH-OH

RN 263167-38-0 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-N,6-dimethyl-5-oxo-N-(2-pyridinylmethyl)-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

10/810,999

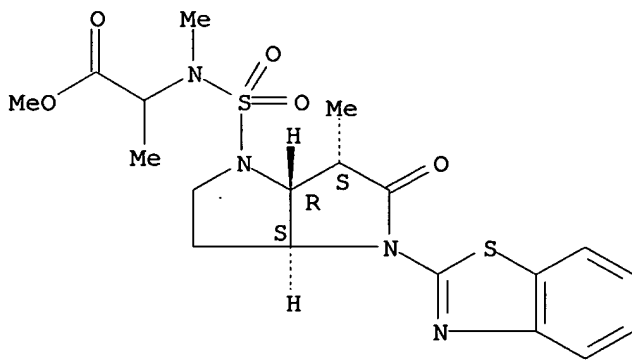
Absolute stereochemistry.



RN 263167-39-1 CAPLUS

CN Alanine, N-[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]-N-methyl-, methyl ester (9CI)
(CA INDEX NAME)

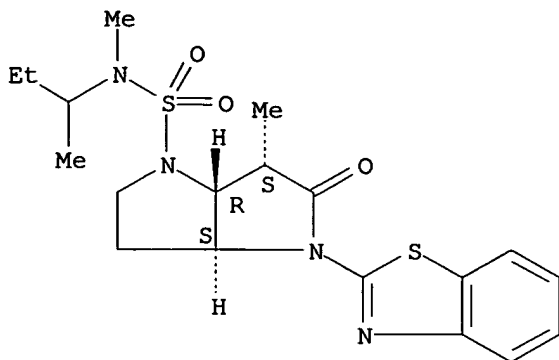
Absolute stereochemistry.



RN 263167-40-4 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(2-benzothiazolyl)hexahydro-N,6-dimethyl-N-(1-methylpropyl)-5-oxo-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

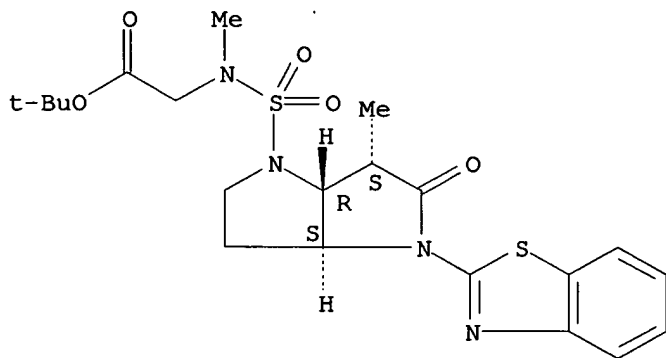
Absolute stereochemistry.



RN 263167-41-5 CAPLUS

CN Glycine, N-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]-N-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

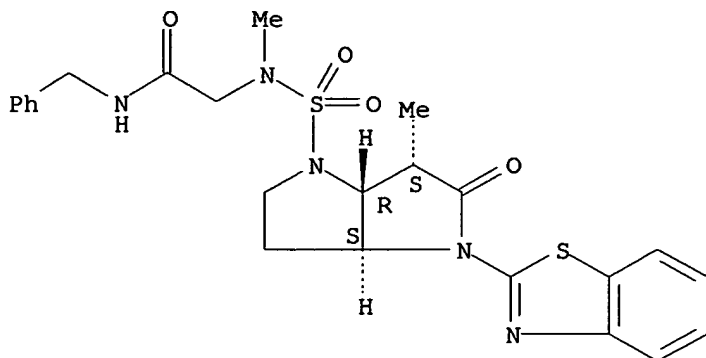
Absolute stereochemistry.



RN 263167-42-6 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

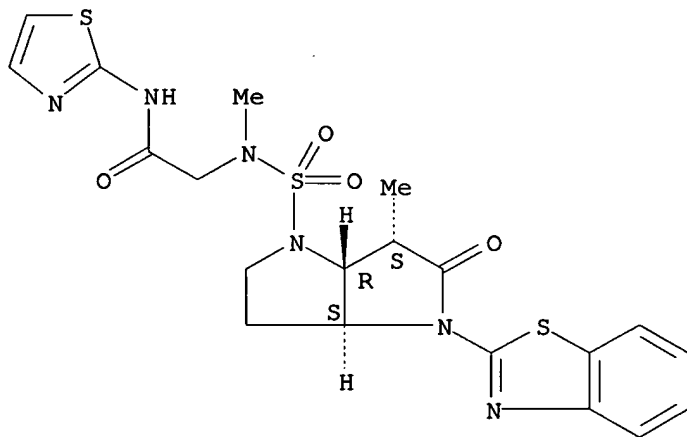
Absolute stereochemistry.



RN 263167-43-7 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-2-thiazolyl- (9CI) (CA INDEX NAME)

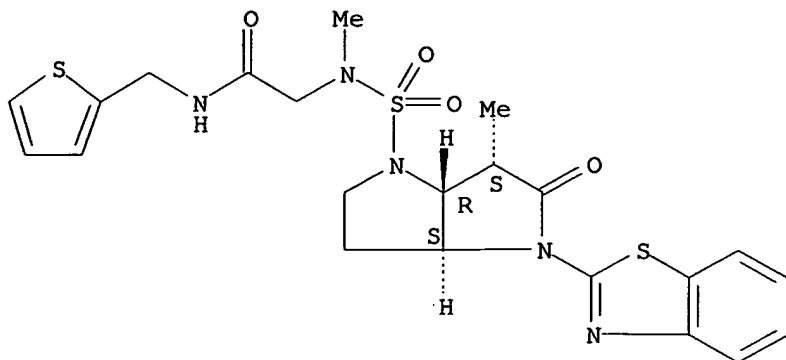
Absolute stereochemistry.



RN 263167-44-8 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(2-thienylmethyl)- (9CI) (CA INDEX NAME)

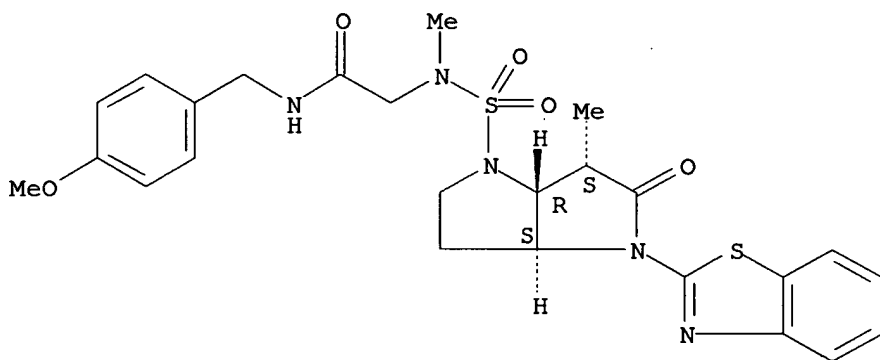
Absolute stereochemistry.



RN 263167-45-9 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

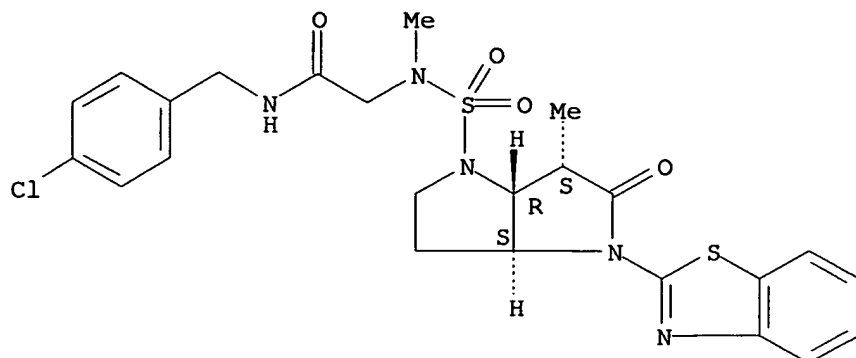
Absolute stereochemistry.



RN 263167-46-0 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(4-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)

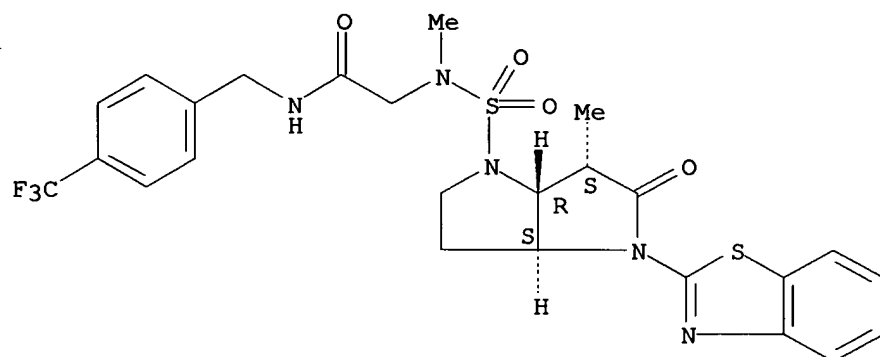
Absolute stereochemistry.



RN 263167-47-1 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

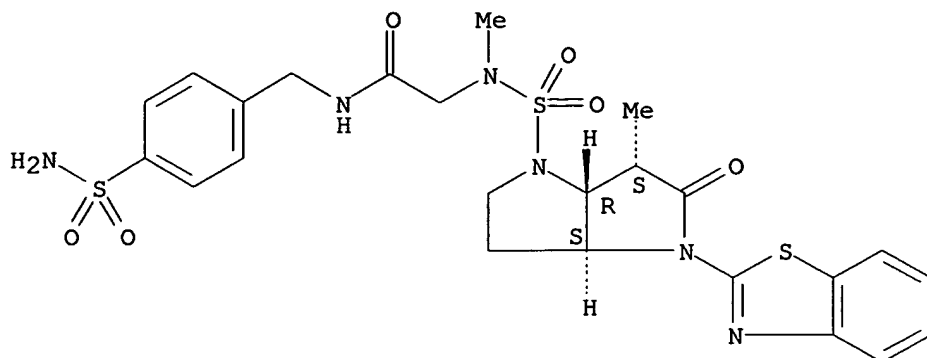
Absolute stereochemistry.



RN 263167-48-2 CAPLUS

CN Acetamide, N-[[4-(aminosulfonyl)phenyl]methyl]-2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]- (9CI) (CA INDEX NAME)

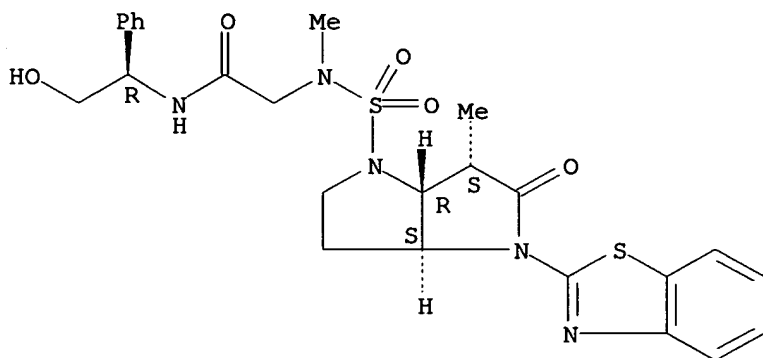
Absolute stereochemistry.



RN 263167-49-3 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(1R)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

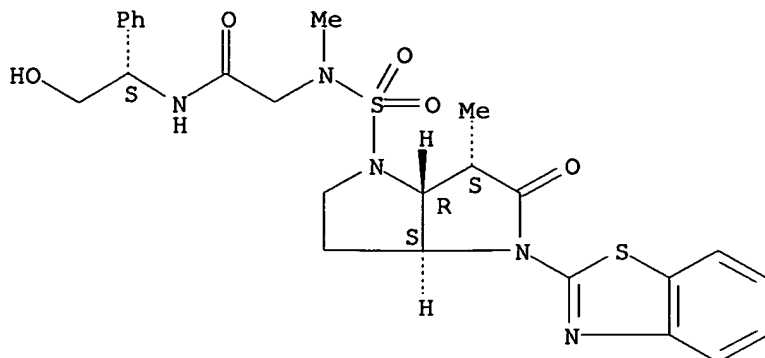
Absolute stereochemistry.



RN 263167-50-6 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

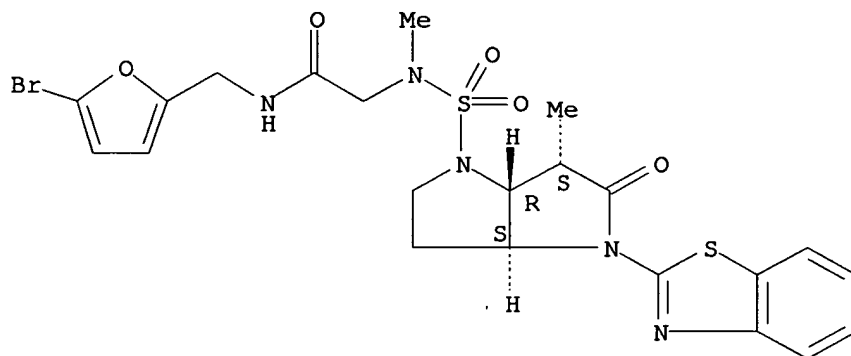
Absolute stereochemistry.



RN 263167-51-7 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(5-bromo-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

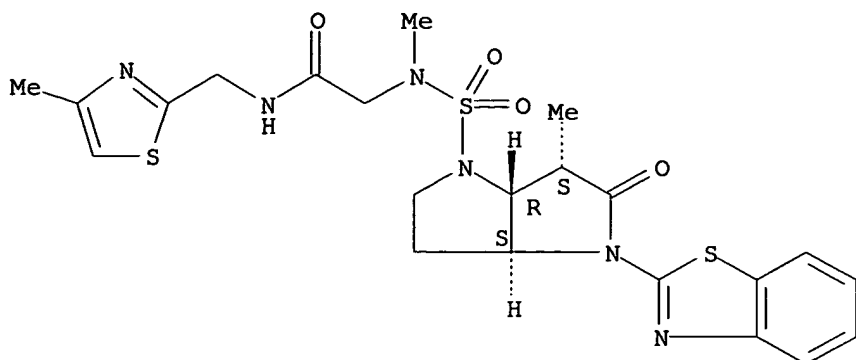
Absolute stereochemistry.



RN 263167-52-8 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(4-methyl-2-thiazolyl)methyl]- (9CI) (CA INDEX NAME)

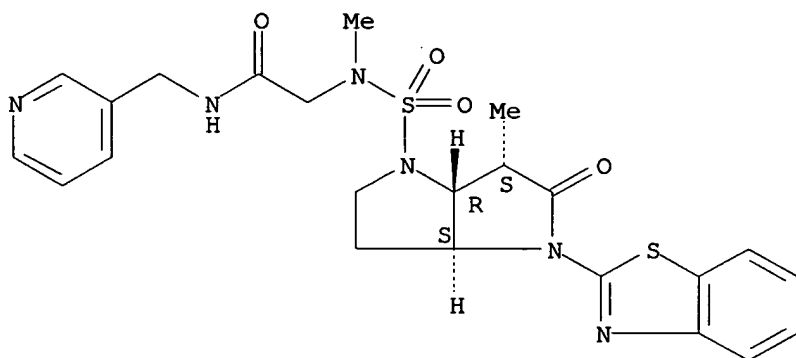
Absolute stereochemistry.



RN 263167-53-9 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

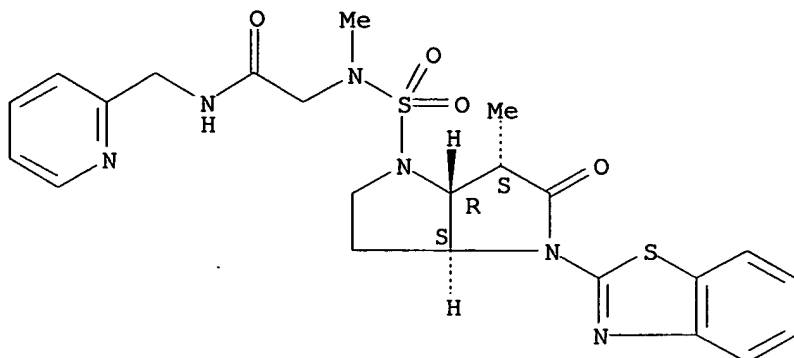
Absolute stereochemistry.



RN 263167-54-0 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)

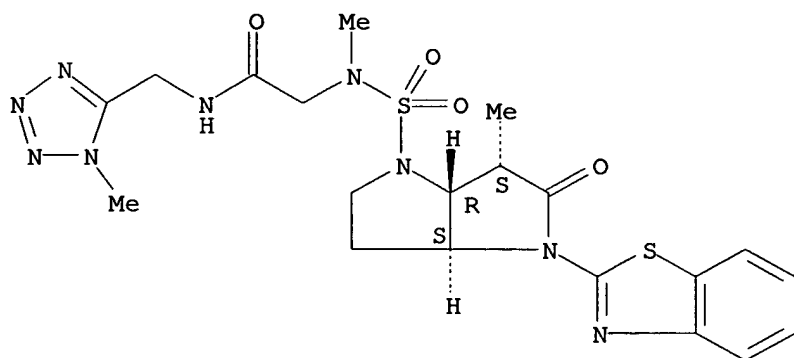
Absolute stereochemistry.



RN 263167-55-1 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(1-methyl-1H-tetrazol-5-yl)methyl]- (9CI) (CA INDEX NAME)

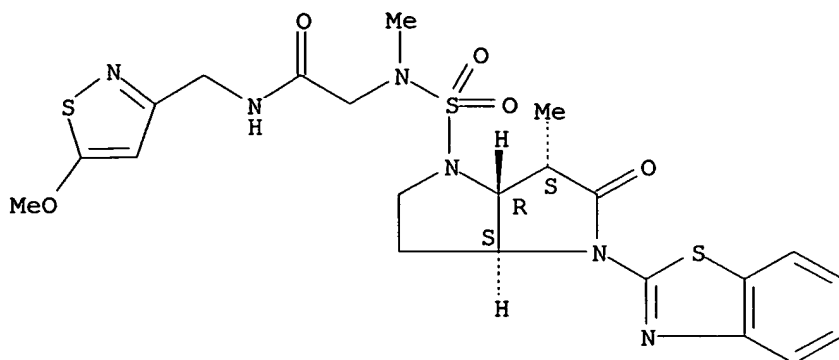
Absolute stereochemistry.



RN 263167-56-2 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(5-methoxy-3-isothiazolyl)methyl]- (9CI) (CA INDEX NAME)

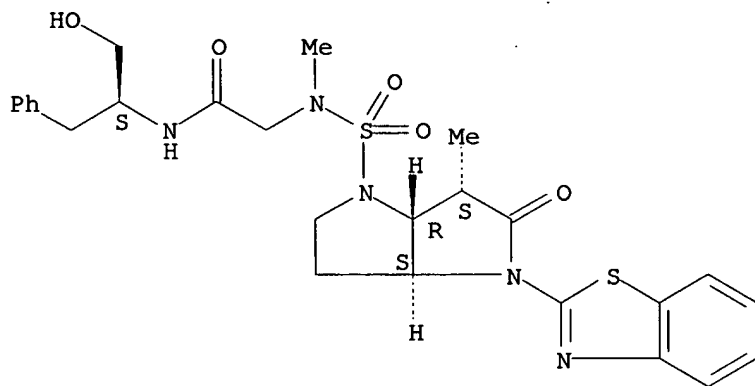
Absolute stereochemistry.



RN 263167-57-3 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]- (9CI) (CA INDEX NAME)

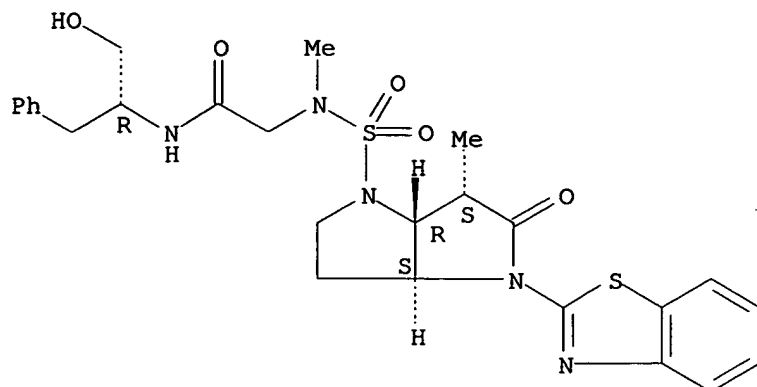
Absolute stereochemistry.



RN 263167-58-4 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(1R)-1-(hydroxymethyl)-2-phenylethyl]- (9CI) (CA INDEX NAME)

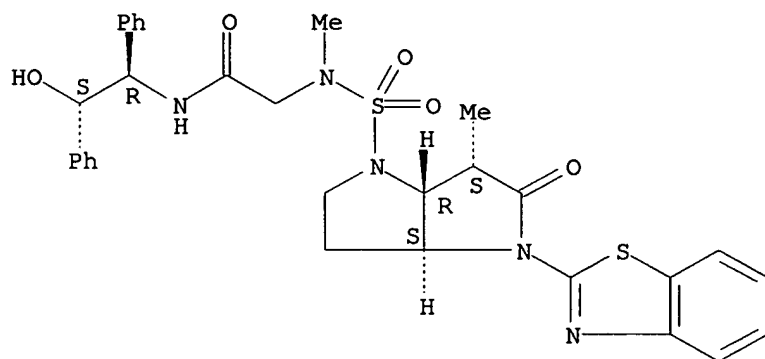
Absolute stereochemistry.



RN 263167-59-5 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(1R,2S)-2-hydroxy-1,2-diphenylethyl]- (9CI) (CA INDEX NAME)

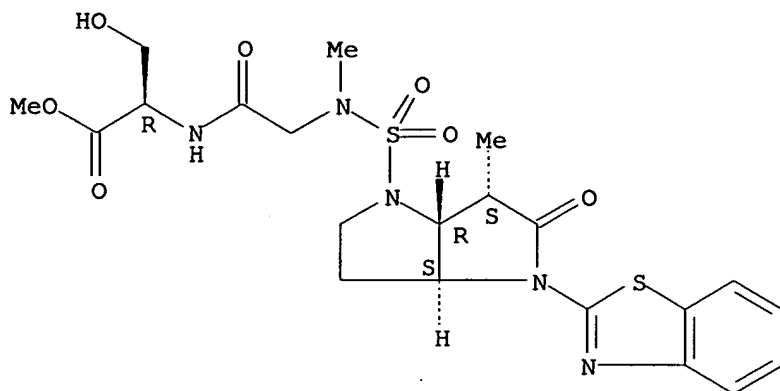
Absolute stereochemistry.



RN 263167-60-8 CAPLUS

CN D-Serine, N-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]-N-methylglycyl-, methyl ester (9CI) (CA INDEX NAME)

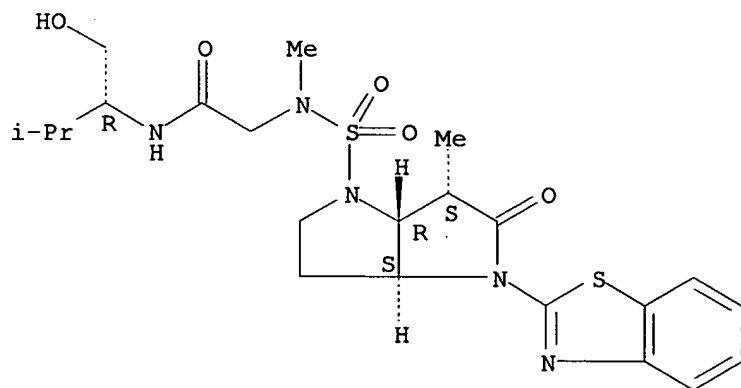
Absolute stereochemistry.



RN 263167-61-9 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(1R)-1-(hydroxymethyl)-2-methylpropyl]- (9CI) (CA INDEX NAME)

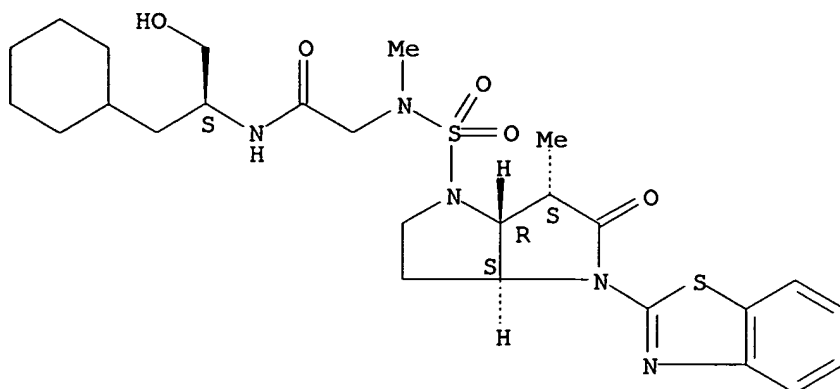
Absolute stereochemistry.



RN 263167-62-0 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(1S)-2-cyclohexyl-1-(hydroxymethyl)ethyl]- (9CI) (CA INDEX NAME)

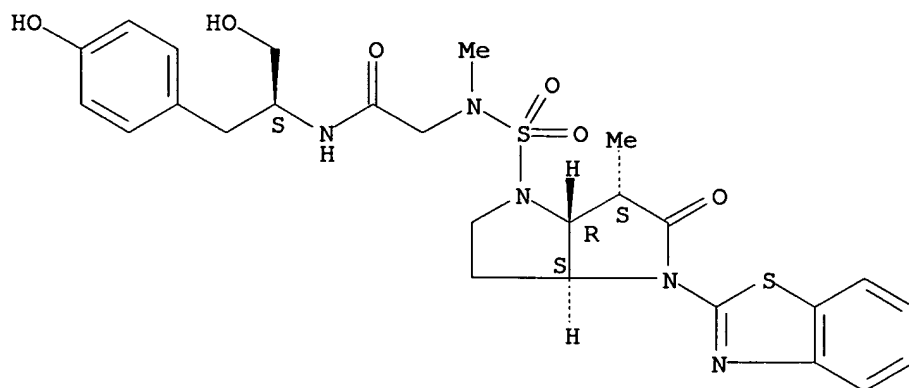
Absolute stereochemistry.



RN 263167-63-1 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-[(1S)-2-hydroxy-1-[(4-hydroxyphenyl)methyl]ethyl]- (9CI) (CA INDEX NAME)

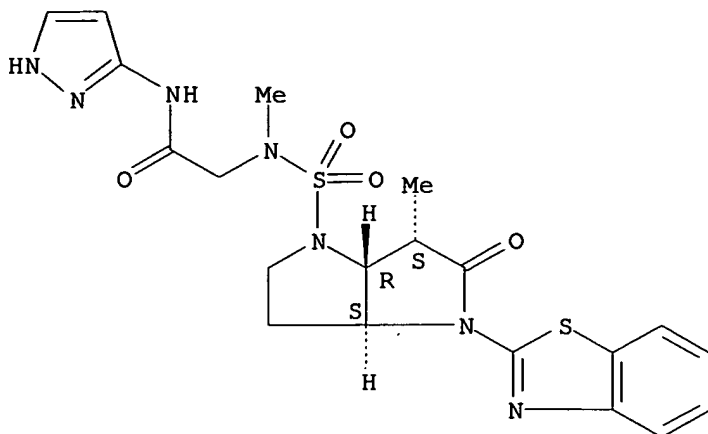
Absolute stereochemistry.



RN 263167-64-2 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-1H-pyrazol-3-yl- (9CI) (CA INDEX NAME)

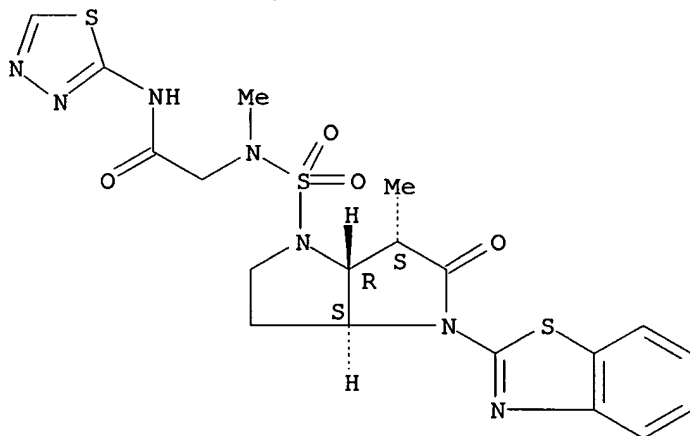
Absolute stereochemistry.



RN 263167-65-3 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-1,3,4-thiadiazol-2-yl- (9CI) (CA INDEX NAME)

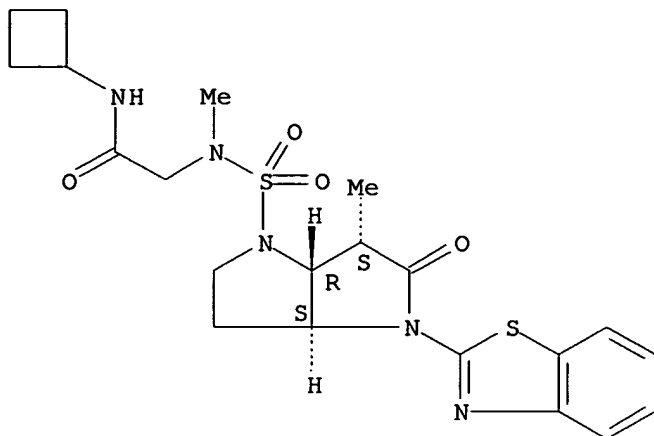
Absolute stereochemistry.



RN 263167-66-4 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-cyclobutyl- (9CI) (CA INDEX NAME)

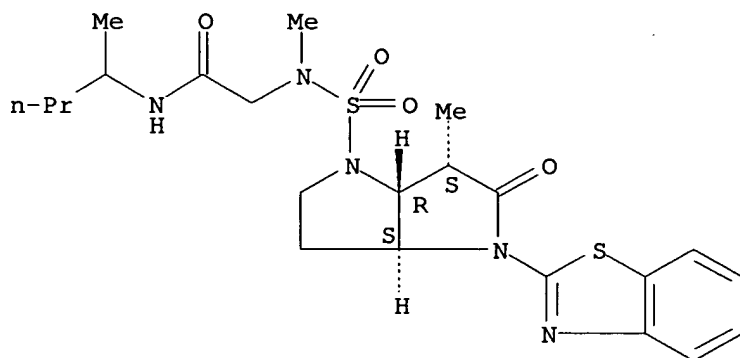
Absolute stereochemistry.



RN 263167-67-5 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(1-methylbutyl)-(9CI) (CA INDEX NAME)

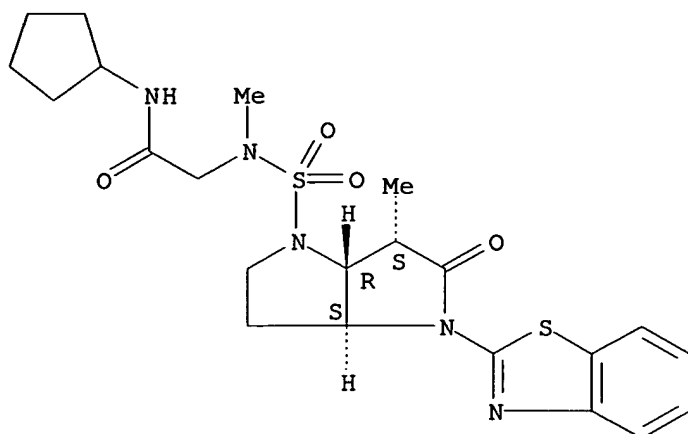
Absolute stereochemistry.



RN 263167-68-6 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-cyclopentyl-(9CI) (CA INDEX NAME)

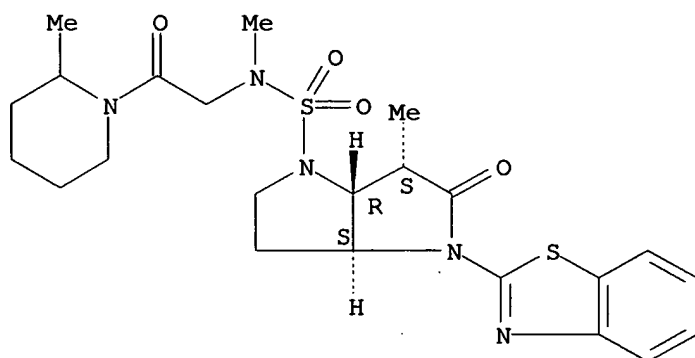
Absolute stereochemistry.



RN 263167-69-7 CAPLUS

CN Piperidine, 1-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]acetyl]-2-methyl- (9CI) (CA INDEX NAME)

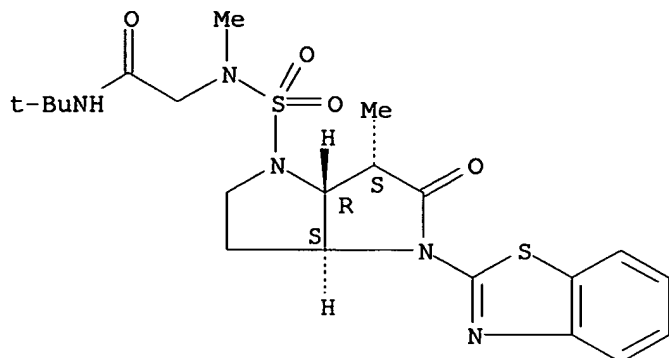
Absolute stereochemistry.



RN 263167-70-0 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

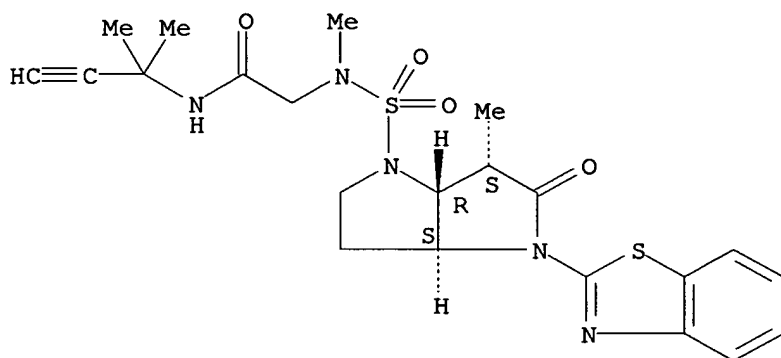
Absolute stereochemistry.



RN 263167-71-1 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(1,1-dimethyl-2-propynyl)- (9CI) (CA INDEX NAME)

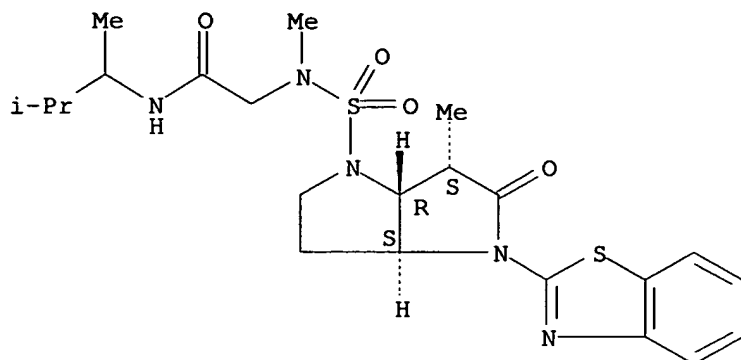
Absolute stereochemistry.



RN 263167-72-2 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(1,2-dimethylpropyl)- (9CI) (CA INDEX NAME)

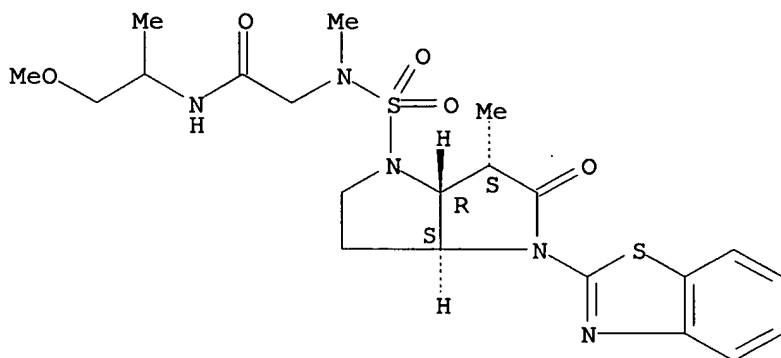
Absolute stereochemistry.



RN 263167-73-3 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(2-methoxy-1-methylethyl)- (9CI) (CA INDEX NAME)

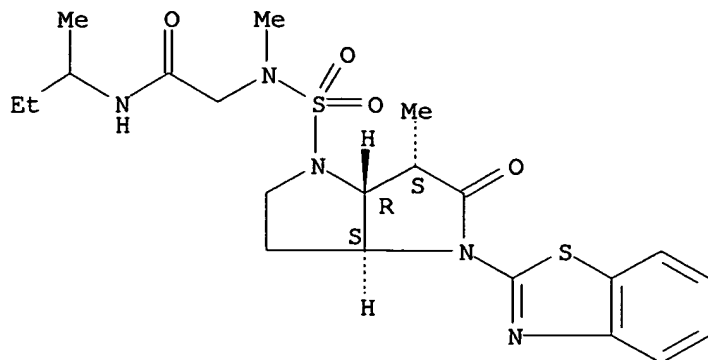
Absolute stereochemistry.



RN 263167-74-4 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-(1-methylpropyl)- (9CI) (CA INDEX NAME)

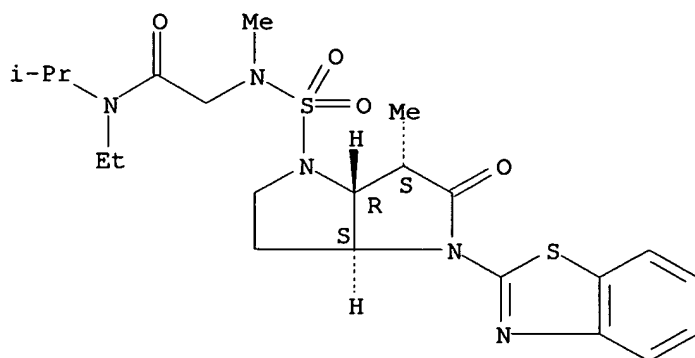
Absolute stereochemistry.



RN 263167-75-5 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-ethyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

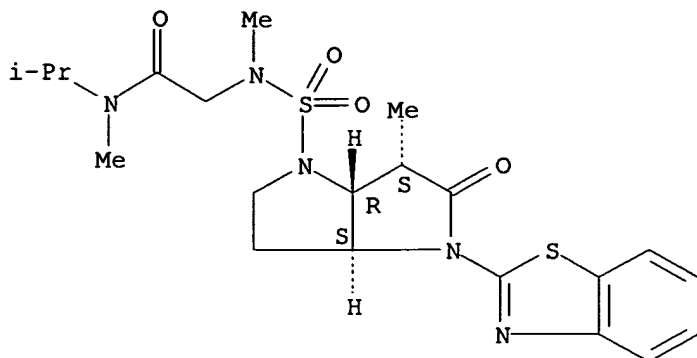
Absolute stereochemistry.



RN 263167-76-6 CAPLUS

CN Acetamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-N-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

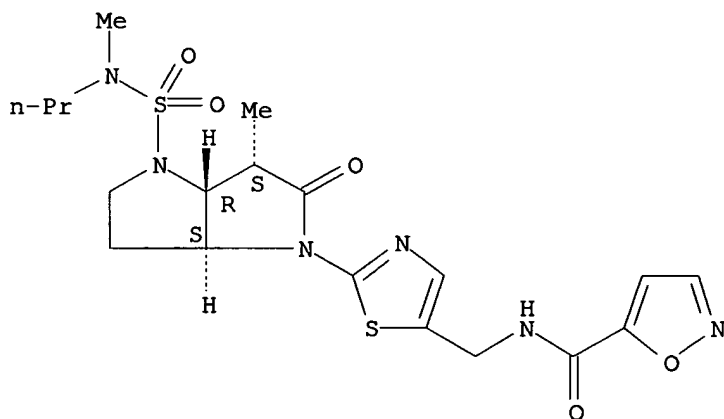
Absolute stereochemistry.



RN 263167-88-0 CAPLUS

CN 5-Isoxazolecarboxamide, N-[[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

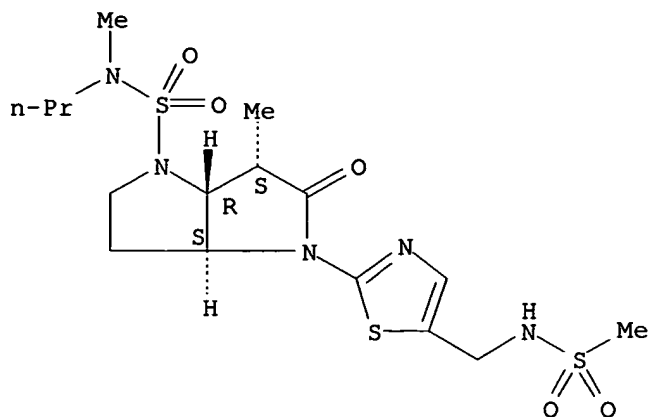
Absolute stereochemistry.



RN 263167-89-1 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-N,6-dimethyl-4-[5-[[[(methylsulfonyl)amino]methyl]-2-thiazolyl]-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

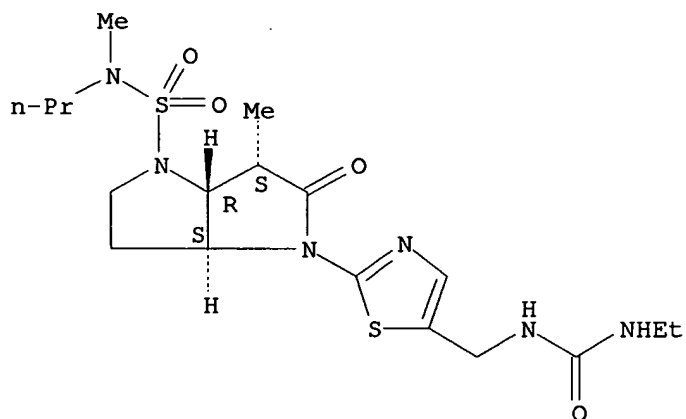
Absolute stereochemistry.



RN 263167-90-4 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[5-
[[[(ethylamino)carbonyl]amino]methyl]-2-thiazolyl]hexahydro-N,6-dimethyl-5-
oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

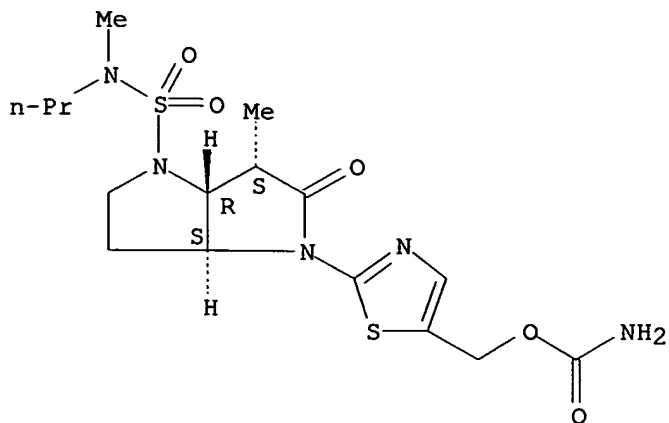
Absolute stereochemistry.



RN 263167-91-5 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[5-[[[(aminocarbonyl)oxy]methyl]-
2-thiazolyl]methyl]amino]methyl]-2-thiazolyl]hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI)
(CA INDEX NAME)

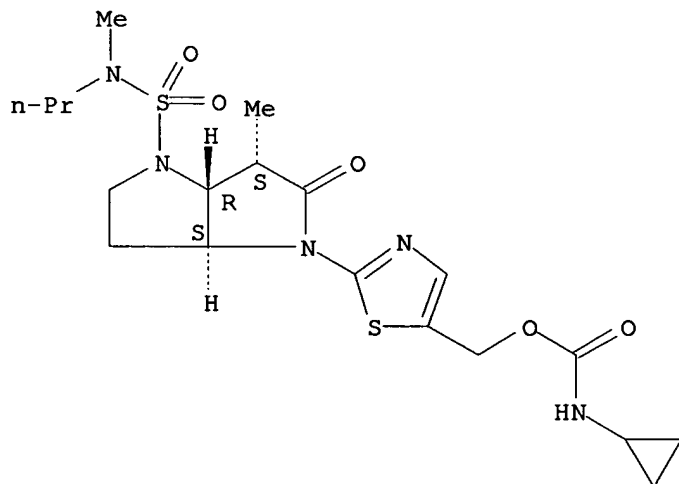
Absolute stereochemistry.



RN 263167-92-6 CAPLUS

CN Carbamic acid, cyclopropyl-, [2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

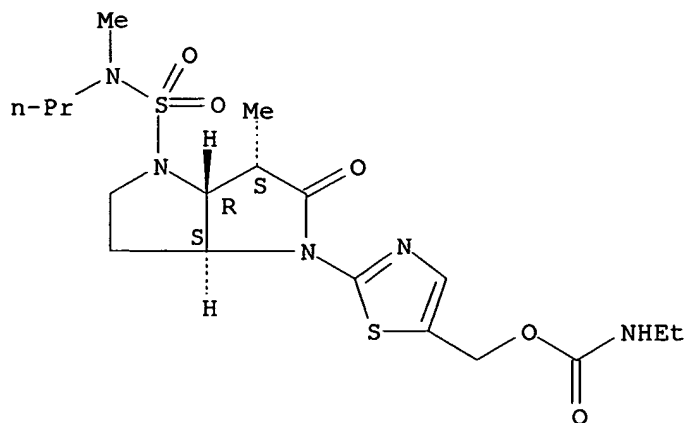
Absolute stereochemistry.



RN 263167-93-7 CAPLUS

CN Carbamic acid, ethyl-, [2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

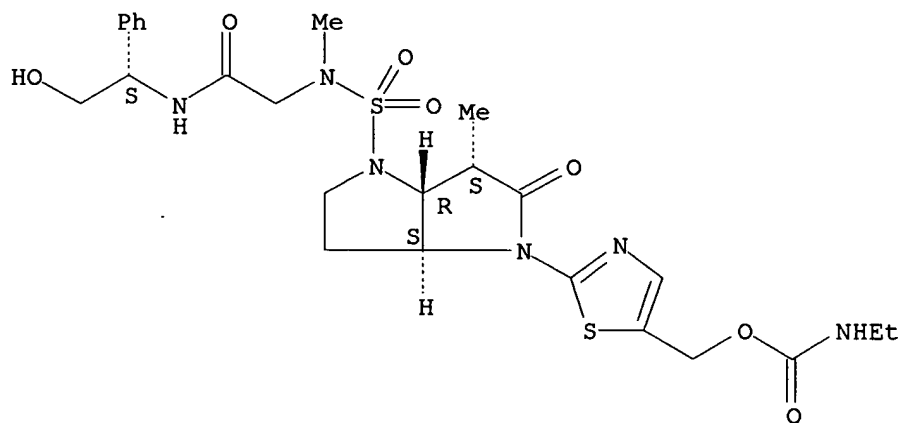
Absolute stereochemistry.



RN 263167-95-9 CAPLUS

CN Carbamic acid, ethyl-, [2-[(3S,3aR,6aS)-hexahydro-4-[[[2-[(1S)-2-hydroxy-1-phenylethyl]amino]-2-oxoethyl]methylamino]sulfonyl]-3-methyl-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

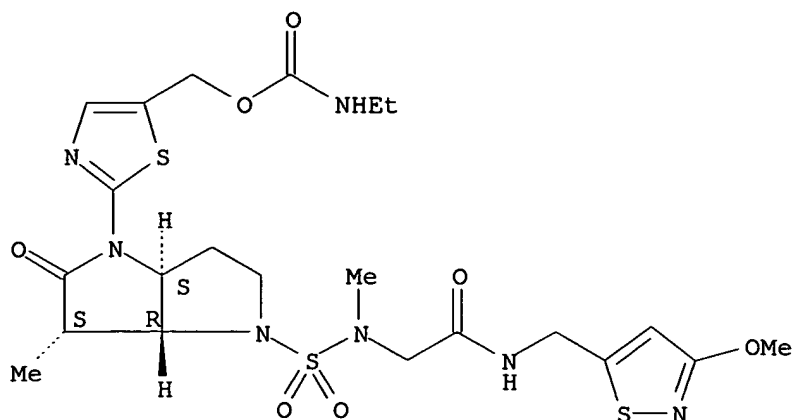
Absolute stereochemistry.



RN 263167-96-0 CAPLUS

CN Carbamic acid, ethyl-, [2-[(3S,3aR,6aS)-hexahydro-4-[[[2-[(3-methoxy-5-isothiazolyl)methyl]amino]-2-oxoethyl]methylamino]sulfonyl]-3-methyl-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

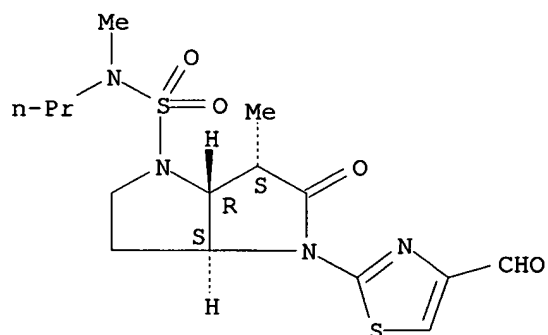
Absolute stereochemistry.



RN 263167-98-2 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(4-formyl-2-thiazolyl)hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

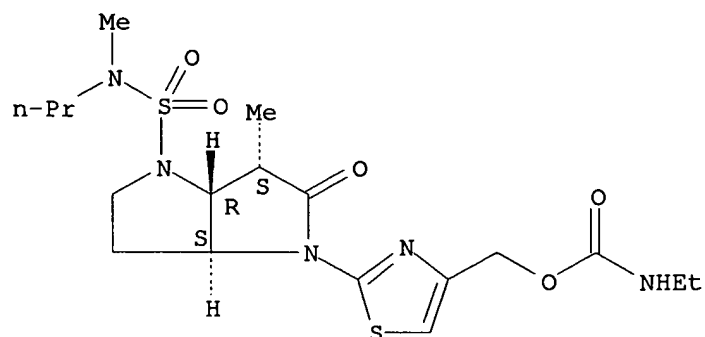
Absolute stereochemistry.



RN 263167-99-3 CAPLUS

CN Carbamic acid, ethyl-, [2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-4-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

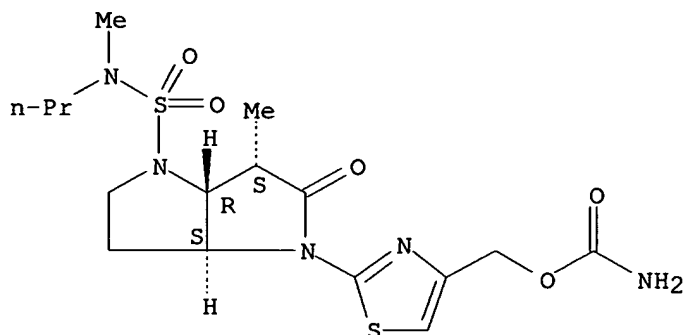
Absolute stereochemistry.



RN 263168-00-9 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[4-[[(aminocarbonyl)oxy]methyl]-2-thiazolyl]hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)-(9CI)
(CA INDEX NAME)

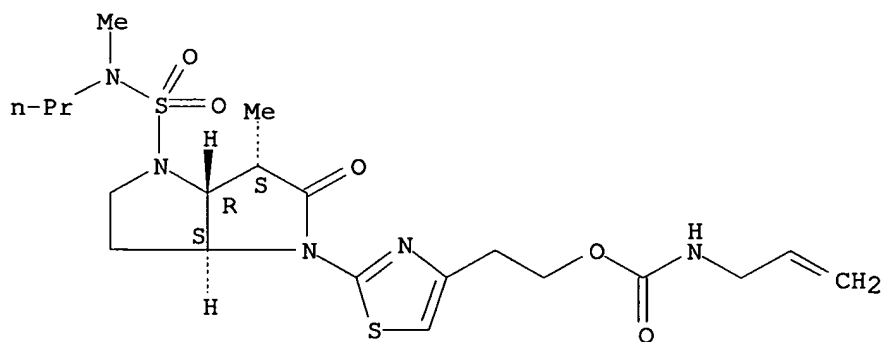
Absolute stereochemistry.



RN 263168-02-1 CAPLUS

CN Carbamic acid, 2-propenyl-, 2-[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-4-thiazolyl]ethyl ester (9CI) (CA INDEX NAME)

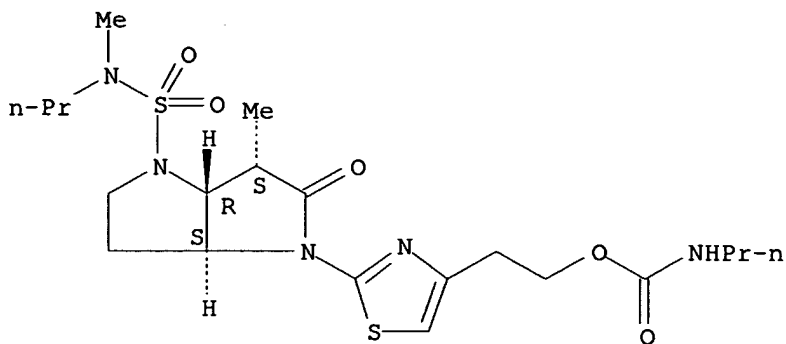
Absolute stereochemistry.



RN 263168-03-2 CAPLUS

CN Carbamic acid, propyl-, 2-[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-4-thiazolyl]ethyl ester (9CI) (CA INDEX NAME)

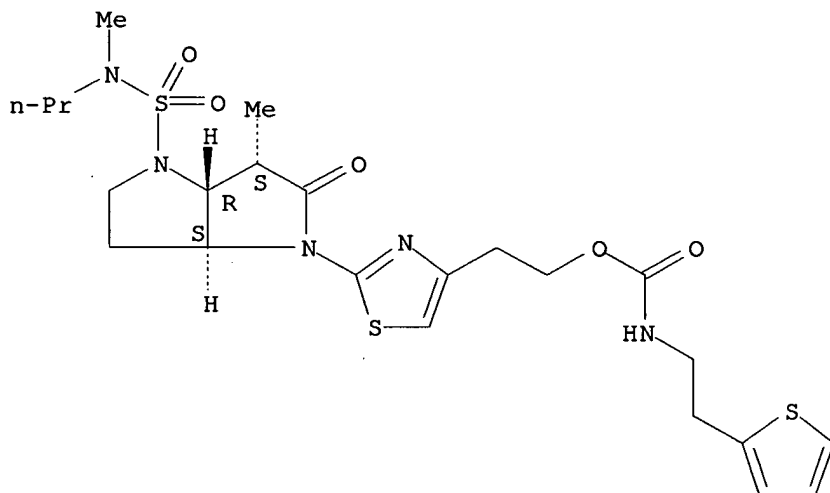
Absolute stereochemistry.



RN 263168-04-3 CAPLUS

CN Carbamic acid, [2-(2-thienyl)ethyl]-, 2-[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-4-thiazolyl]ethyl ester (9CI) (CA INDEX NAME)

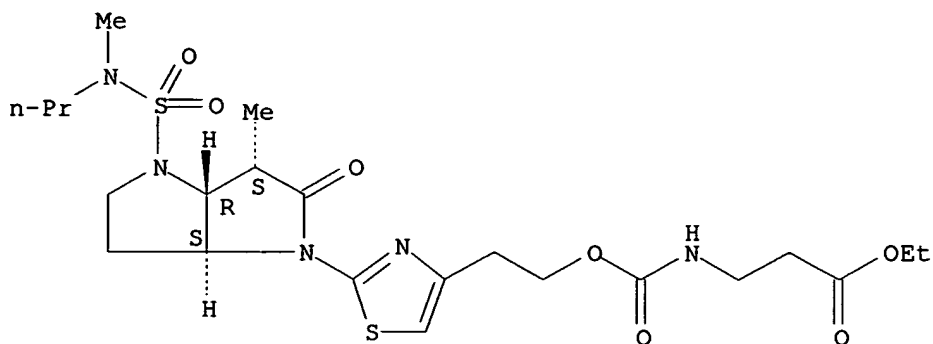
Absolute stereochemistry.



RN 263168-05-4 CAPLUS

CN β -Alanine, N-[[2-[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-4-thiazolyl]ethoxy]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

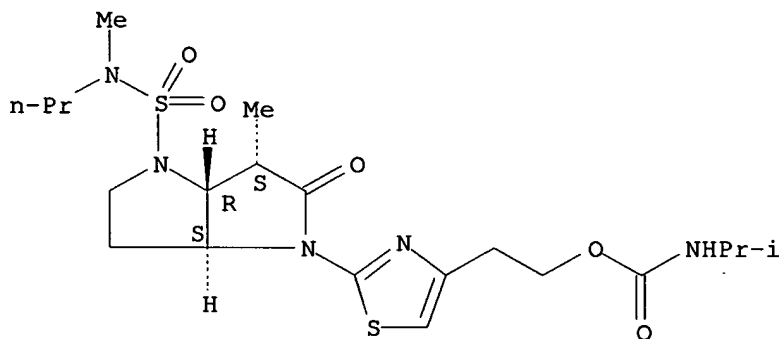
Absolute stereochemistry.



RN 263168-06-5 CAPLUS

CN Carbamic acid, (1-methylethyl)-, 2-[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-4-thiazolyl]ethyl ester (9CI) (CA INDEX NAME)

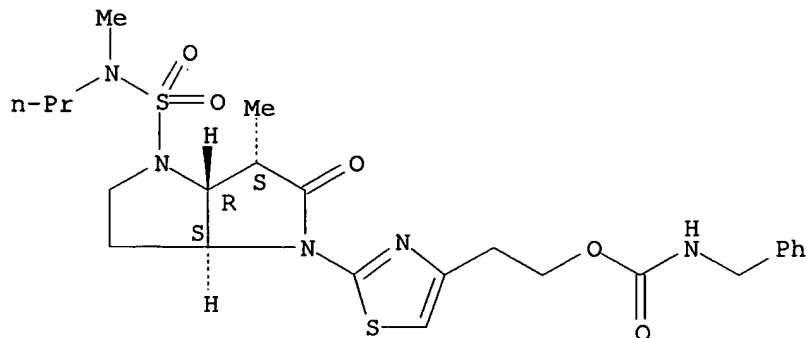
Absolute stereochemistry.



RN 263168-07-6 CAPLUS

CN Carbamic acid, (phenylmethyl)-, 2-[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-4-thiazolyl]ethyl ester (9CI) (CA INDEX NAME)

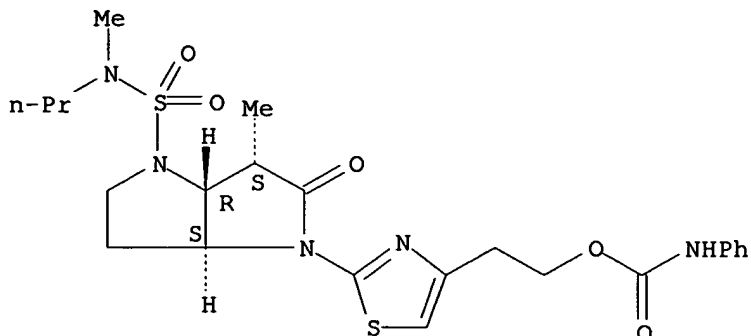
Absolute stereochemistry.



RN 263168-08-7 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-N,6-dimethyl-5-oxo-4-[4-[2-[[(phenylamino)carbonyl]oxy]ethyl]-2-thiazolyl]-N-propyl-, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

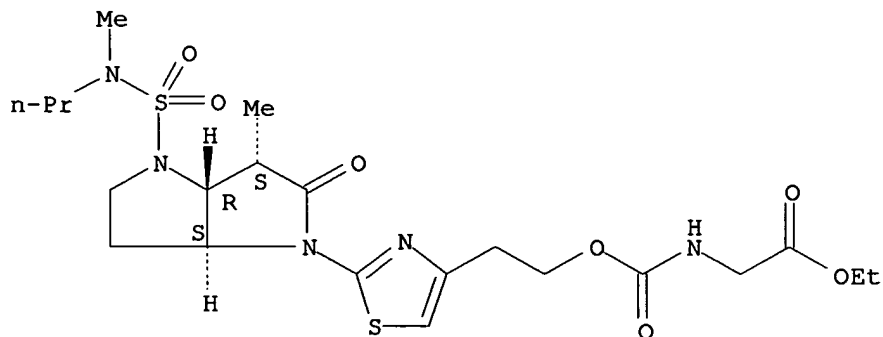
Absolute stereochemistry.



RN 263168-09-8 CAPLUS

CN Glycine, N-[[2-[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-4-thiazolyl]ethoxy]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

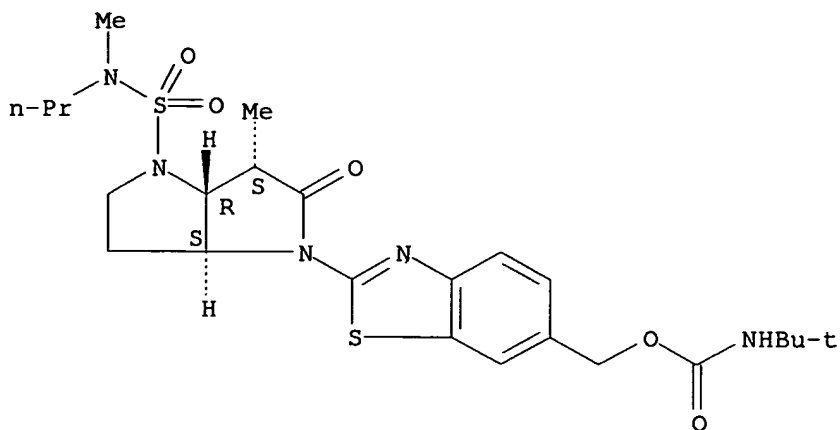
Absolute stereochemistry.



RN 263168-11-2 CAPLUS

CN Carbamic acid, (1,1-dimethylethyl)-, [2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-6-benzothiazolyl]methyl ester (9CI) (CA INDEX NAME)

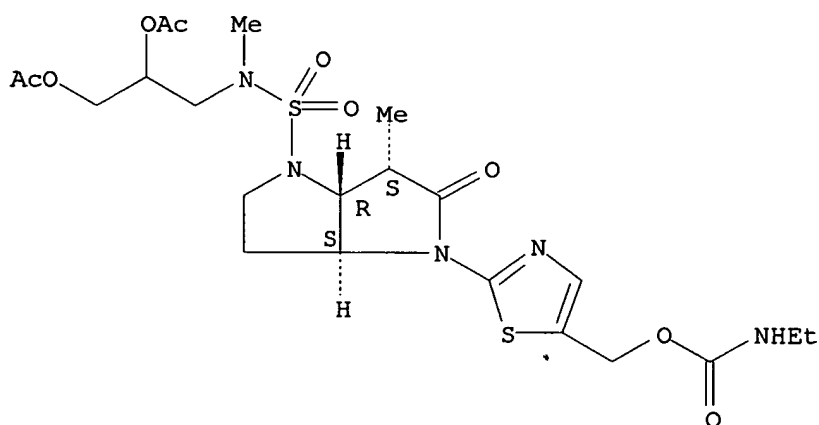
Absolute stereochemistry.



RN 263168-15-6 CAPLUS

CN Carbamic acid, ethyl-, [2-[(3S,3aR,6aS)-4-[[[2,3-bis(acetyloxy)propyl]methylamino]sulfonyl]hexahydro-3-methyl-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

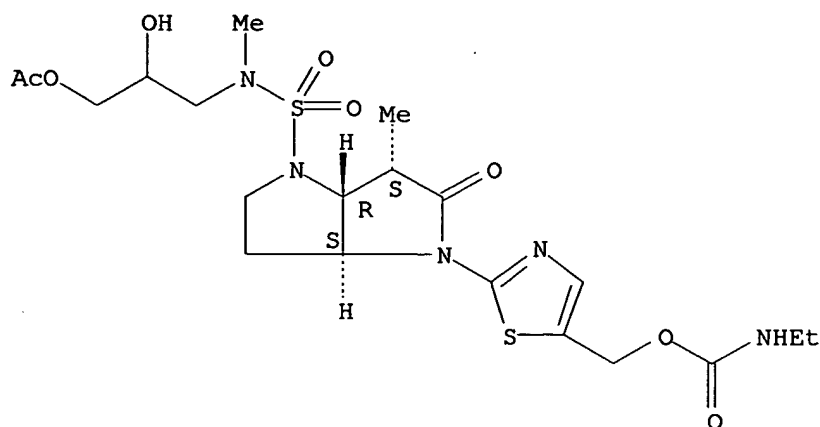
Absolute stereochemistry.



RN 263168-16-7 CAPLUS

CN Carbamic acid, ethyl-, [2-[(3S,3aR,6aS)-4-[[[3-(acetyloxy)-2-hydroxypropyl]methylamino]sulfonyl]hexahydro-3-methyl-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

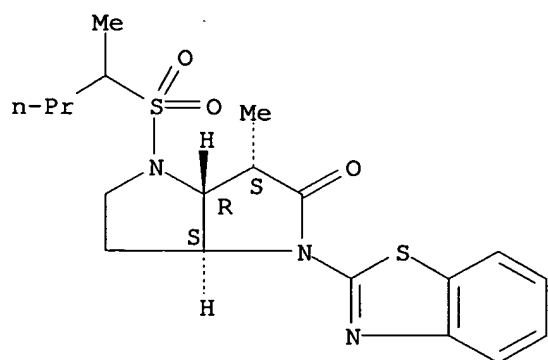
Absolute stereochemistry.



RN 263168-83-8 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)hexahydro-3-methyl-4-[(1-methylbutyl)sulfonyl]-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

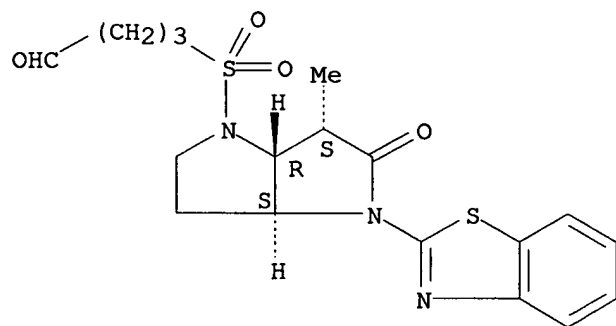
Absolute stereochemistry.



RN 263168-85-0 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)hexahydro-3-methyl-4-[(4-oxobutyl)sulfonyl]-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

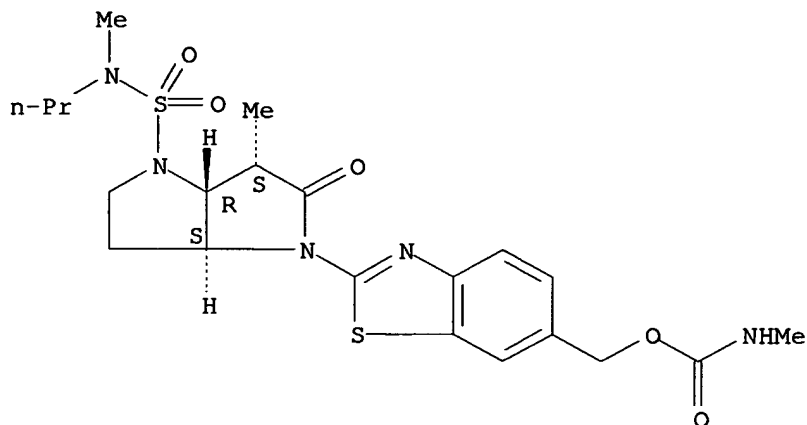


10/810,999

RN 263168-86-1 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, hexahydro-N,6-dimethyl-4-[6-
[[[(methylamino)carbonyl]oxy]methyl]-2-benzothiazolyl]-5-oxo-N-propyl-,
(3aS,6S,6aR)- (9CI) (CA INDEX NAME)

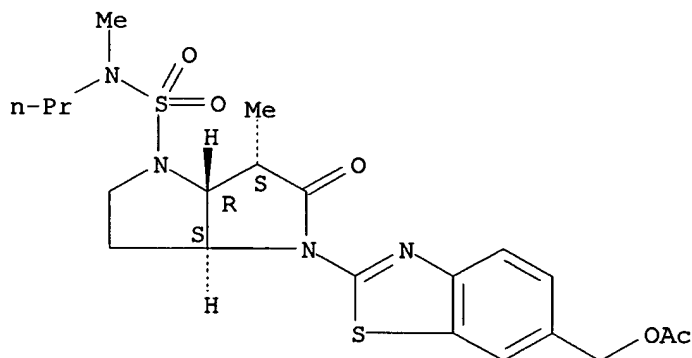
Absolute stereochemistry.



RN 263168-87-2 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-[6-[(acetyloxy)methyl]-2-
benzothiazolyl]hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI)
(CA INDEX NAME)

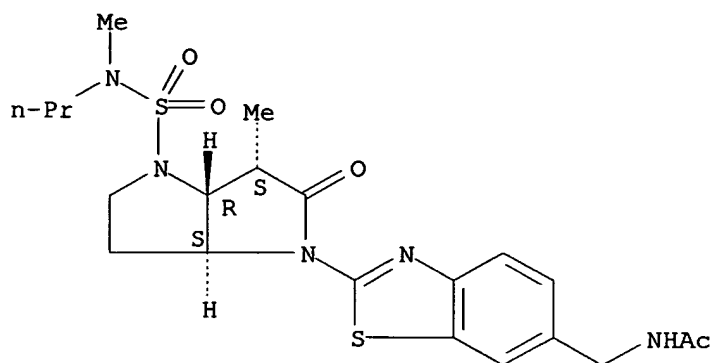
Absolute stereochemistry.



RN 263168-88-3 CAPLUS

CN Acetamide, N-[[2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-
[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-6-
benzothiazolyl]methyl]- (9CI) (CA INDEX NAME)

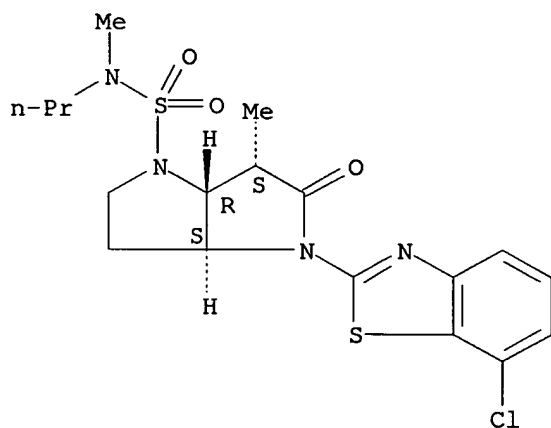
Absolute stereochemistry.



RN 263168-89-4 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-sulfonamide, 4-(7-chloro-2-benzothiazolyl)hexahydro-N,6-dimethyl-5-oxo-N-propyl-, (3aS,6S,6aR)- (9CI)
(CA INDEX NAME)

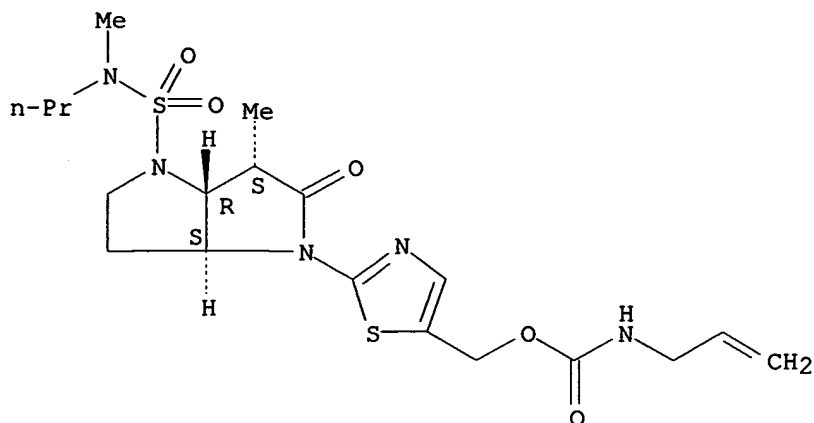
Absolute stereochemistry.



RN 263168-90-7 CAPLUS

CN Carbamic acid, 2-propenyl-, [2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

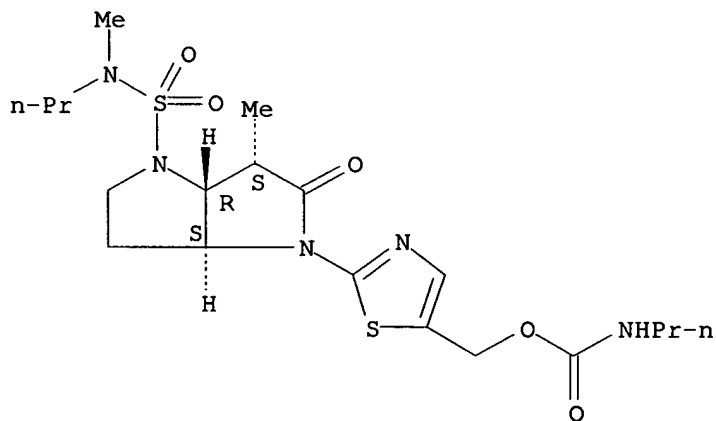
Absolute stereochemistry.



RN 263168-91-8 CAPLUS

CN Carbamic acid, propyl-, [2-[(3S,3aR,6aS)-hexahydro-3-methyl-4-[(methylpropylamino)sulfonyl]-2-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]-5-thiazolyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263168-93-0 CAPLUS

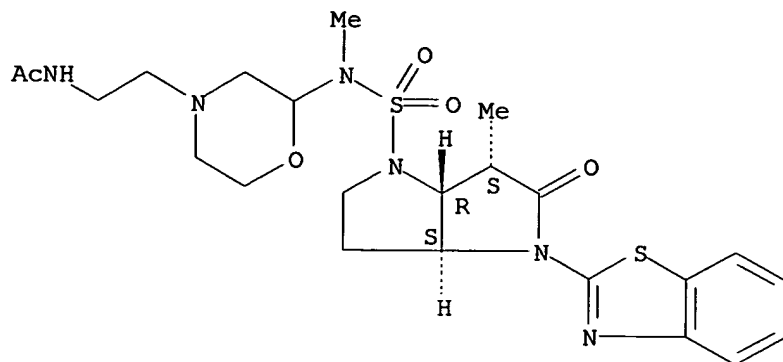
CN Formic acid, compd. with N-[2-[2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]sulfonyl]methylamino]-4-morpholinyl]ethyl]acetamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 263168-92-9

CMF C23 H32 N6 O5 S2

Absolute stereochemistry.



CM 2

CRN 64-18-6

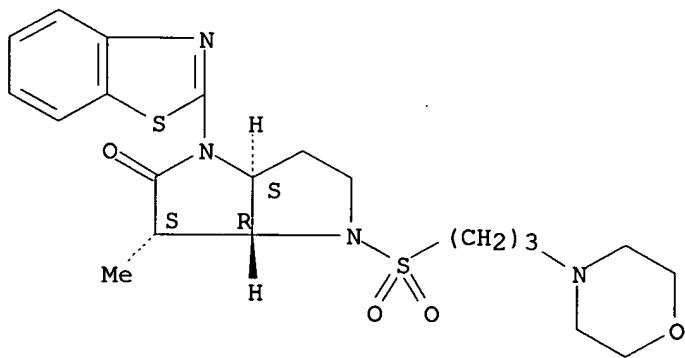
CMF C H2 O2

O=CH-OH

RN 263169-66-0 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)hexahydro-3-methyl-4-[[3-(4-morpholinyl)propyl]sulfonyl]-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

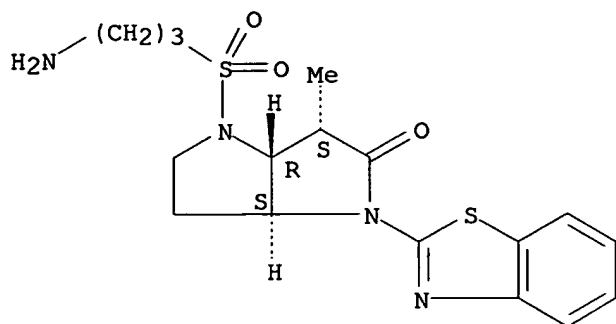


RN 263169-67-1 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 4-[(3-aminopropyl)sulfonyl]-1-(2-benzothiazolyl)hexahydro-3-methyl-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/810,999



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/810,999

110 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:572661 CAPLUS

DOCUMENT NUMBER: 131:351212

TITLE: Synthesis and antimicrobial activity of
4H-4-oxoquinolizine derivatives: consequences of
structural modification at the C-8 position

AUTHOR(S): Ma, Zhenkun; Chu, Daniel T. W.; Cooper, Curt S.; Li,
Qun; Fung, Anthony K. L.; Wang, Sanyi; Shen, Linus L.;
Flamm, Robert K.; Nilius, Angela M.; Alder, Jeffery
D.; Meulbroek, Jonathan A.; Or, Yat Sun

CORPORATE SOURCE: Infectious Disease Research, Abbott Laboratories,
Abbott Park, IL, 60064-3537, USA

SOURCE: Journal of Medicinal Chemistry (1999), 42(20),
4202-4213

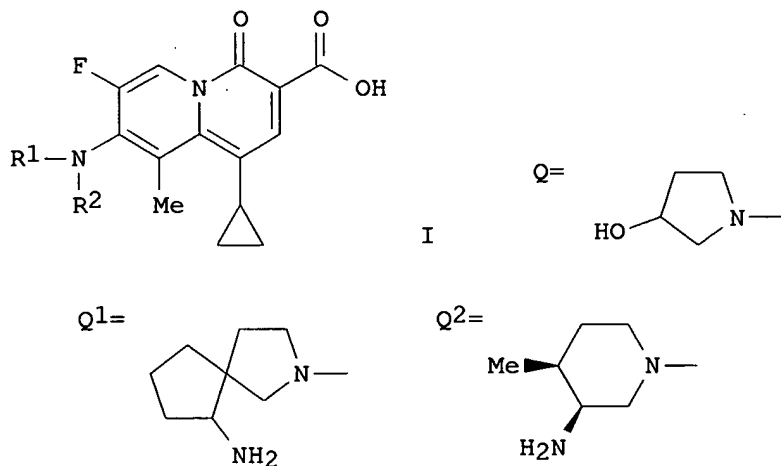
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The antibacterial 4H-4-oxoquinolizines were introduced recently to overcome bacterial resistance to fluoroquinolones. They exhibit potent antibacterial activity against Gram-pos., Gram-neg., and anaerobic organisms and are highly active against some quinolone-resistant bacteria including quinolone-resistant MRSA. Preliminary studies indicated that oxoquinolizines possess distinct activity and toxicity profiles as compared with their parent quinolones. In order to develop a potent antibacterial agent with the desired spectrum of activity, good tolerability, and balanced pharmacokinetic profile, the authors synthesized and evaluated a series of oxoquinolizines with various substituents at the C-8 position I (NR¹R² = Q, Q¹, Q², etc.). Most compds. tested in this study demonstrated better activity against Gram-pos. bacteria than ciprofloxacin and exhibited good susceptibility against ciprofloxacin- and methicillin-resistant *S. aureus*. While maintaining potent in vitro activity, several compds. showed improved in vivo efficacy over ABT-719 as indicated by the mouse protection test. The current study revealed that the steric and electronic environment, conformation, and absolute stereochem. of the C-8 group are very important to

the antibacterial profiles. Structural modifications of the C-8 group provide a useful means to improve the antibacterial activities, physicochem. properties, and pharmacokinetic profiles. Manipulation of the C-8 group also allows us to generate analogs with the desired spectrum of activity, such as analogs that are selective against respiratory pathogens.

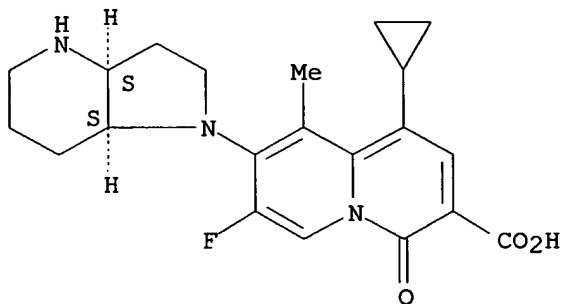
IT 250274-76-1P 250274-77-2P 250274-78-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, structure, bactericidal activity, and structure-activity relationship of oxoquinolizines)

RN 250274-76-1 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-[(3aR,7aR)-octahydro-1H-pyrrolo[3,2-b]pyridin-1-yl]-4-oxo-, rel- (9CI) (CA INDEX NAME)

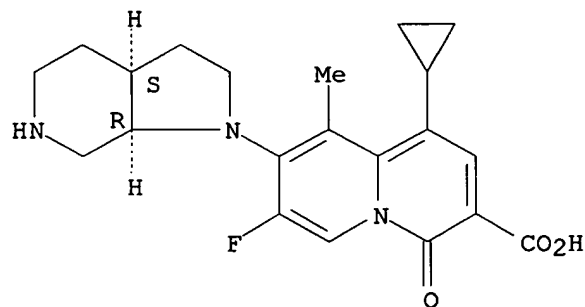
Relative stereochemistry.



RN 250274-77-2 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-[(3aR,7aS)-octahydro-1H-pyrrolo[2,3-c]pyridin-1-yl]-4-oxo-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

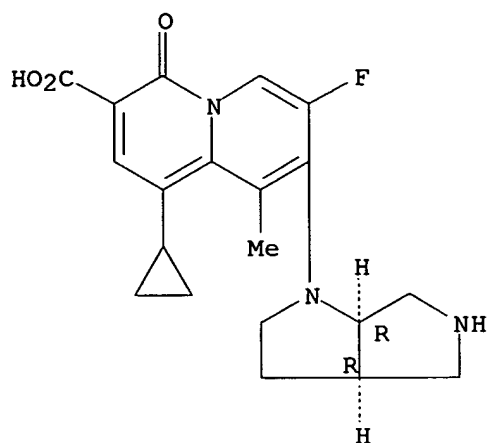
RN 250274-78-3 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aR,6aR)-

10/810,999

hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-9-methyl-4-oxo-, rel- (9CI) (CA
INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

21

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/810,999

~~110~~ ANSWER 17 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:682248 CAPLUS

DOCUMENT NUMBER: 129:302643

TITLE: Preparation of pyrrolopyrrolidinones as antiviral agents

INVENTOR(S): Borthwick, Alan David; Davies, David Evan; Exall, Anne Marjorie; Jackson, Deborah Lynette; Mason, Andrew McMurtrie; Pennell, Andrew Michael Kenneth; Rahim, Saad George; Trivedi, Naimisha; Weingarten, Gordon Gad

PATENT ASSIGNEE(S): Glaxo Group Ltd., UK

SOURCE: PCT Int. Appl., 106 pp.

CODEN: PIXXD2

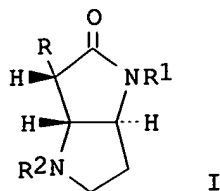
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9843975	A1	19981008	WO 1998-GB982	19980402
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
CA 2286367	AA	19981008	CA 1998-2286367	19980402
AU 9869261	A1	19981022	AU 1998-69261	19980402
EP 973775	A1	20000126	EP 1998-914960	19980402
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2000513013	T2	20001003	JP 1998-541320	19980402
WO 9912932	A1	19990318	WO 1998-EP5607	19980907
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
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AU 9895362	A1	19990329	AU 1998-95362	19980907
ZA 9808160	A	20000322	ZA 1998-8160	19980907
EP 1015454	A1	20000705	EP 1998-948907	19980907
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
JP 2001515903	T2	20010925	JP 2000-510739	19980907
PRIORITY APPLN. INFO.:			GB 1997-6668	A 19970402
			GB 1997-19151	A 19970909
			GB 1997-19189	A 19970909
			WO 1998-GB982	W 19980402
			WO 1998-EP5607	W 19980907
OTHER SOURCE(S):	MARPAT 129:302643			
GI				



AB Title compds. [I; wherein R represents H, substituted or unsubstituted C1-3 alkyl; R1 represents optionally substituted heteroaryl or fused heteroaryl with one to four heteroatoms, R5CO, R5NHCO, R5CS or R5NHCS wherein R5 may be substituted or unsubstituted and represents H, C1-6 alkyl, C1-6 alkenyl, C3-7 cycloalkyl or fused cycloalkyl, heteroaryl or fused heteroaryl containing one to four heteroatoms, aryl or fused aryl, or arylC1-3alkyl; R2 represents R3-X- or R3CO, wherein R3 may be substituted or unsubstituted N containing rings, one or more further heteroatoms; X represents a linker group chosen from C=O, NHC=O, C(=O)C=O, CH=CHCO, CH2CO, CH2 or SO2], salts and solvates are prepared. The invention related to therapeutically active bicyclic compds. in treatment and prophylaxis, particularly of viral infections of the herpes family.

IT 214336-70-6P 214336-71-7P 214336-72-8P

214336-74-0P 214336-75-1P 214336-76-2P

214336-77-3P 214336-79-5P 214336-80-8P

214336-81-9P 214336-82-0P 214336-83-1P

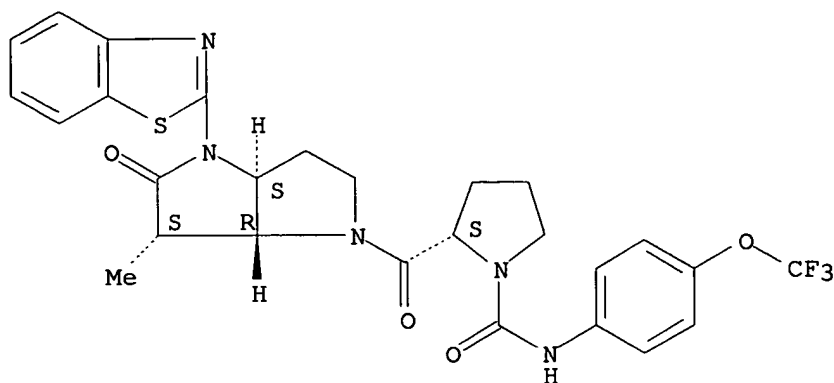
214336-86-4P 214336-90-0P 214336-91-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolopyrrolidinones as antiviral agents)

RN 214336-70-6 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(trifluoromethoxy)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

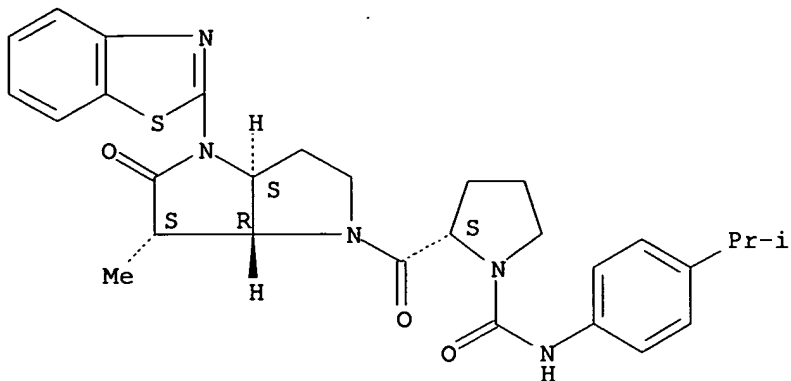
Absolute stereochemistry.



RN 214336-71-7 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

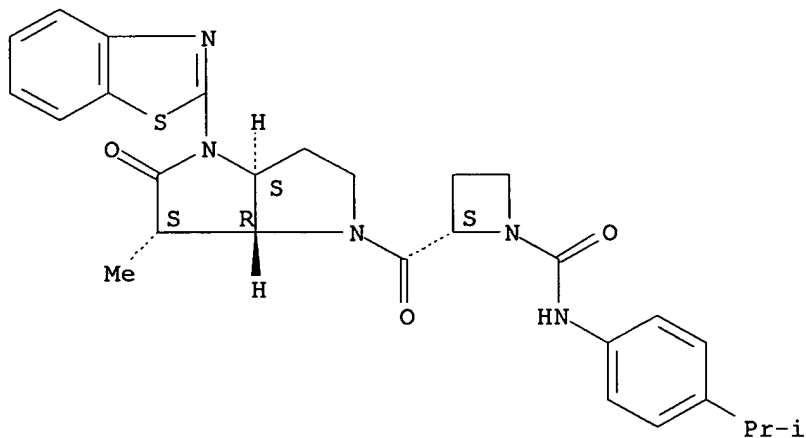
Absolute stereochemistry.



RN 214336-72-8 CAPLUS

CN 1-Azetidinecarboxamide, 2-[[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

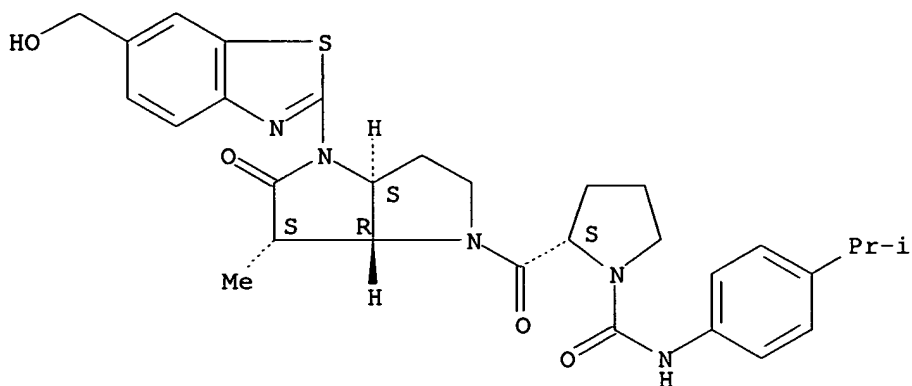
Absolute stereochemistry.



RN 214336-74-0 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-hexahydro-4-[6-(hydroxymethyl)-2-benzothiazolyl]-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

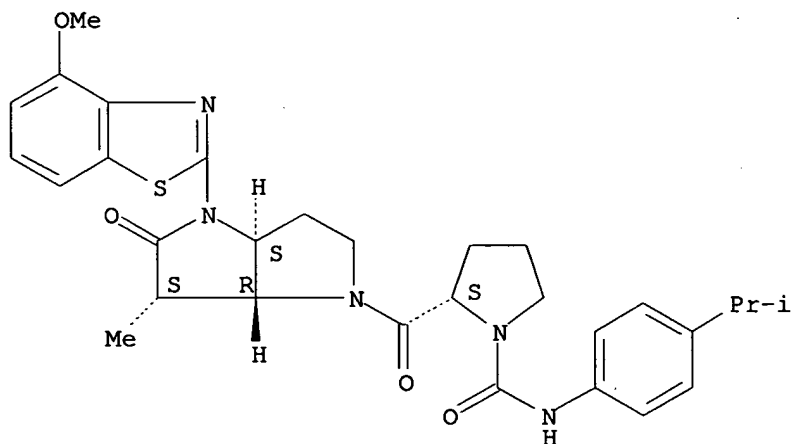
Absolute stereochemistry.



RN 214336-75-1 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aS)-hexahydro-4-(4-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

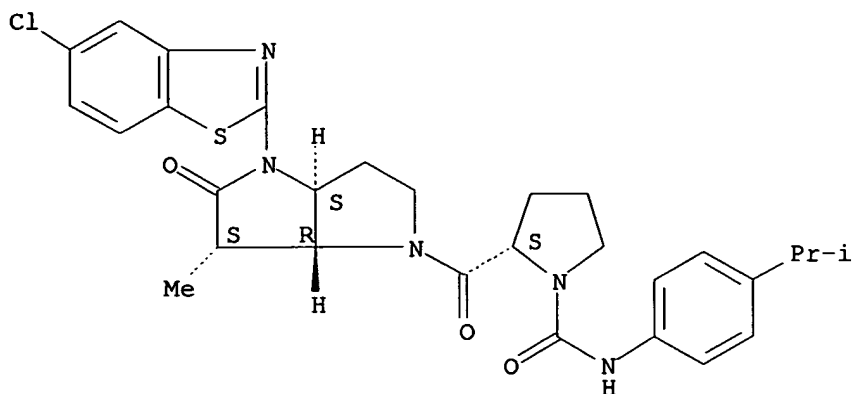
Absolute stereochemistry.



RN 214336-76-2 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-4-(5-chloro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

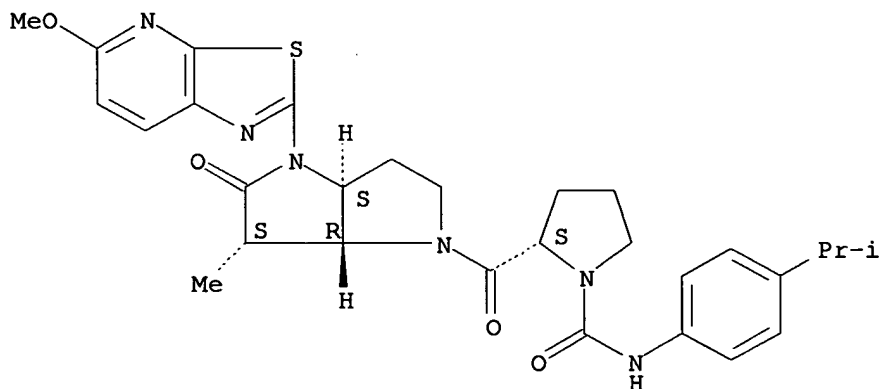
Absolute stereochemistry.



RN 214336-77-3 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-4-(5-methoxythiazolo[5,4-b]pyridin-2-yl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

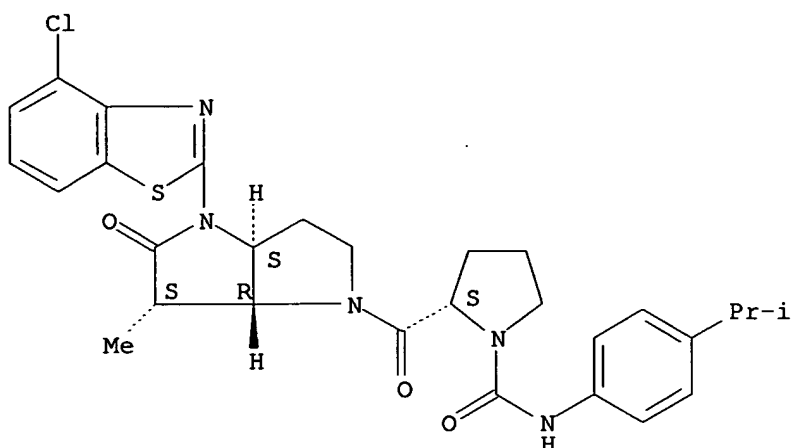
Absolute stereochemistry.



RN 214336-79-5 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aR,6R,6aS)-4-(4-chloro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2R)-rel- (9CI) (CA INDEX NAME)

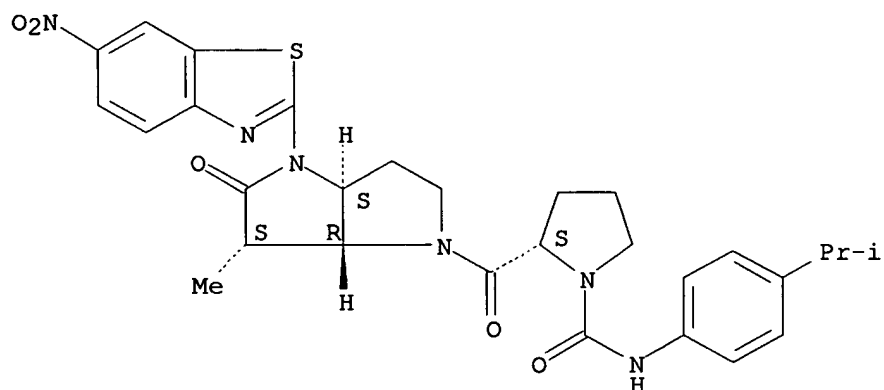
Relative stereochemistry.



RN 214336-80-8 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-hexahydro-6-methyl-4-(6-nitro-2-benzothiazolyl)-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

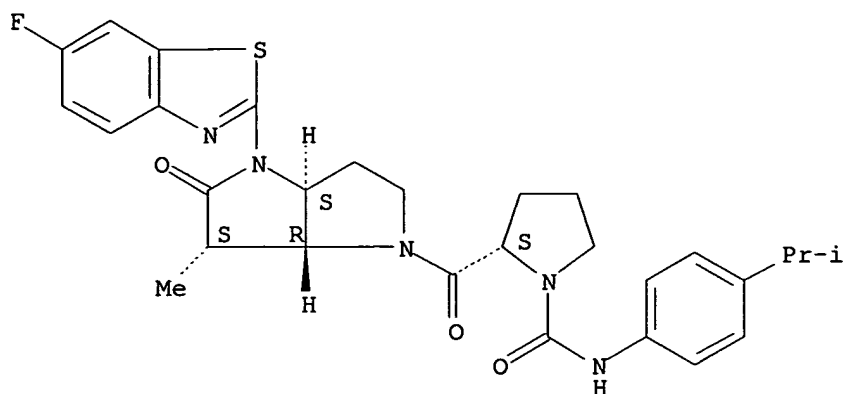
Absolute stereochemistry.



RN 214336-81-9 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-4-(6-fluoro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

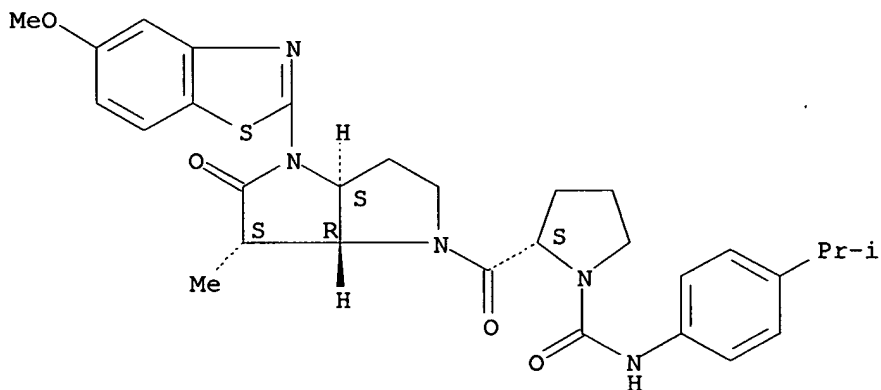
Absolute stereochemistry.



RN 214336-82-0 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-hexahydro-4-(5-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

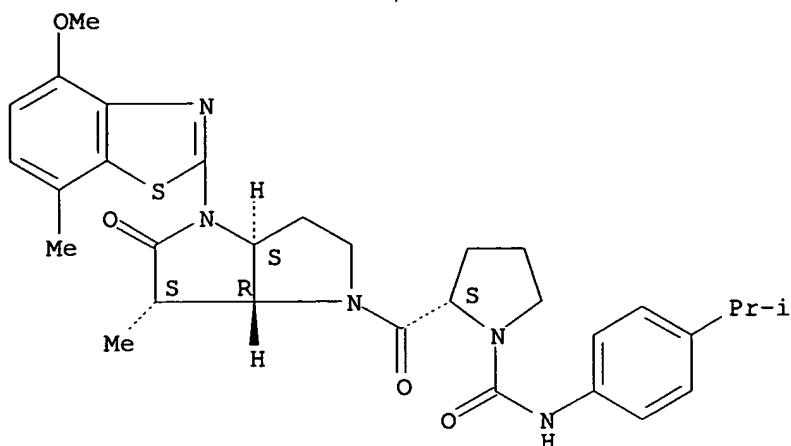
Absolute stereochemistry.



RN 214336-83-1 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[[(3aS,6S,6aR)-hexahydro-4-(4-methoxy-7-methyl-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

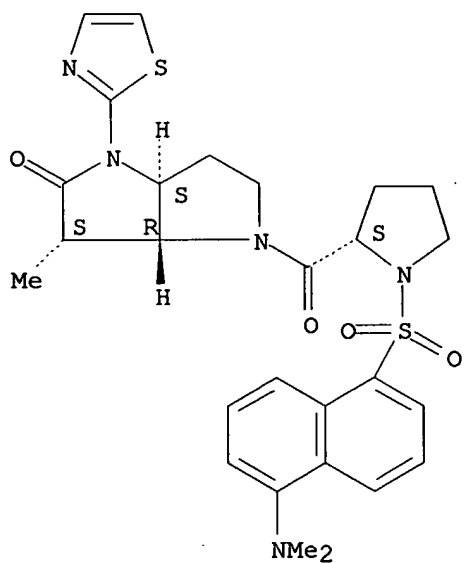
Absolute stereochemistry.



RN 214336-86-4 CAPLUS

CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 4-[[(2S)-1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-2-pyrrolidinyl]carbonyl]hexahydro-3-methyl-1-(2-thiazolyl)-, (3S,3aR,6aS)- (9CI) (CA INDEX NAME)

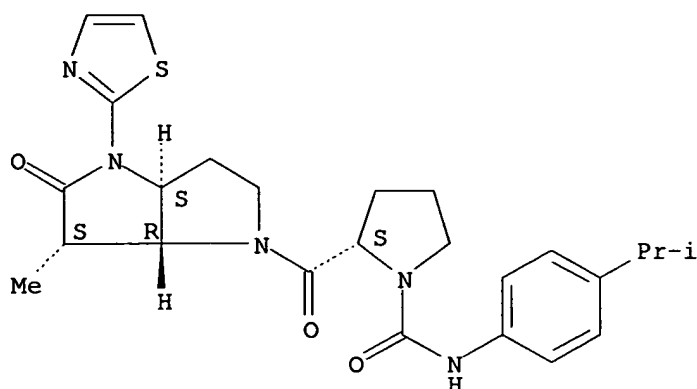
Absolute stereochemistry.



RN 214336-90-0 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-(2-thiazolyl)pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

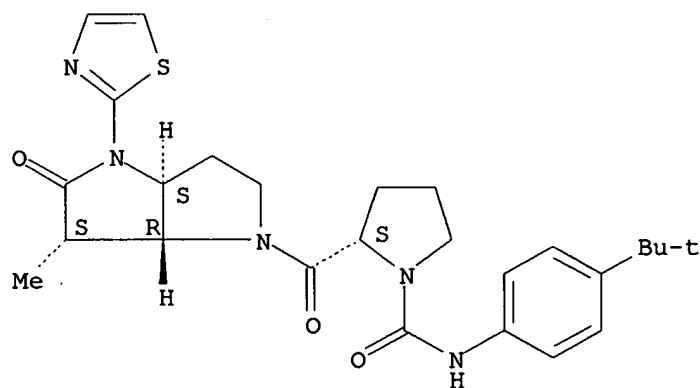
Absolute stereochemistry.



RN 214336-91-1 CAPLUS

CN 1-Pyrrolidinecarboxamide, N-[4-(1,1-dimethylethyl)phenyl]-2-[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-(2-thiazolyl)pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 214337-65-2 214337-66-3 214337-68-5

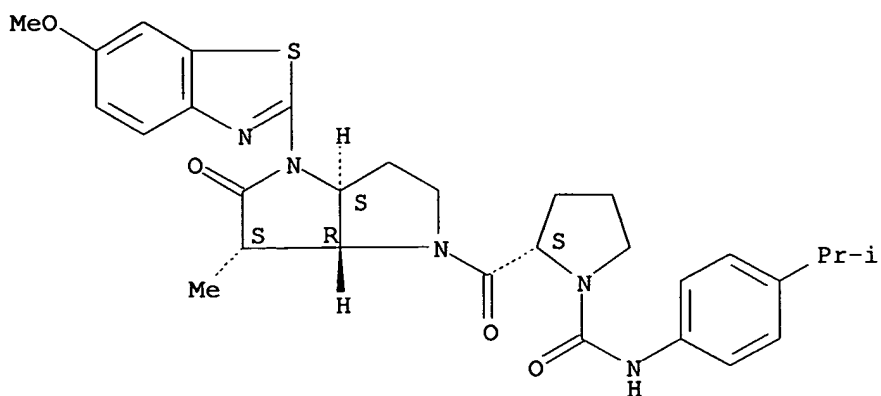
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of pyrrolopyrrolidinones as antiviral agents)

RN 214337-65-2 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-4-(6-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

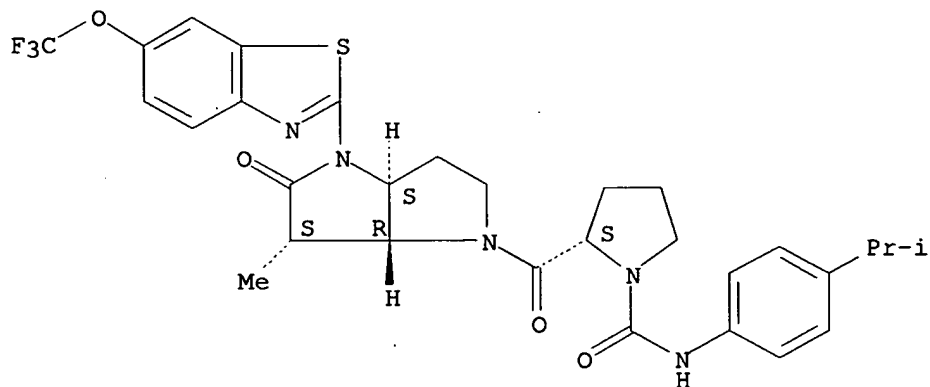
Absolute stereochemistry.



RN 214337-66-3 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-[6-(trifluoromethoxy)-2-benzothiazolyl]pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

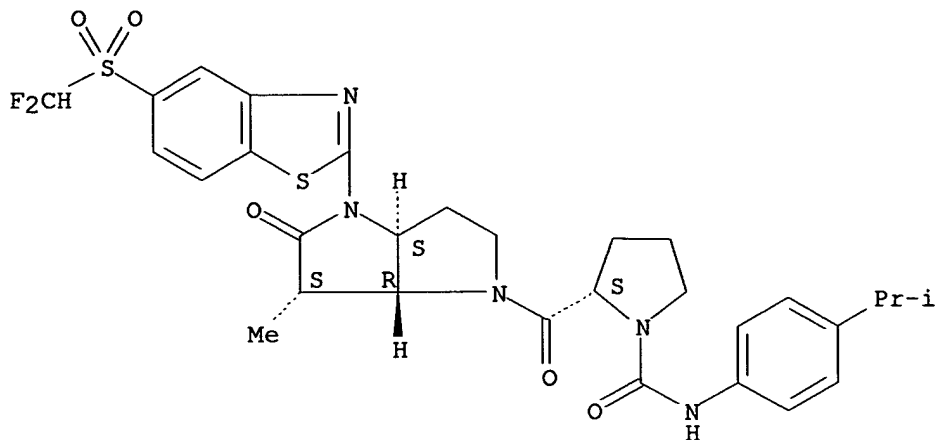
Absolute stereochemistry.



RN 214337-68-5 CAPLUS

CN 1-Pyrrolidinecarboxamide, 2-[[(3aS,6S,6aR)-4-[5-[(difluoromethyl)sulfonyl]-2-benzothiazolyl]hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-N-[4-(1-methylethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 214336-92-2P 214336-94-4P 214337-13-0P
 214337-16-3P 214337-18-5P 214337-26-5P
 214337-31-2P 214337-32-3P 214337-33-4P
 214337-37-8P 214337-41-4P 214337-43-6P
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 214337-52-7P 214337-54-9P 214337-55-0P
 214337-57-2P

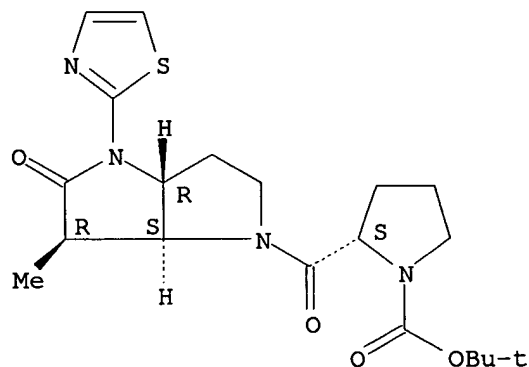
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrrolopyrrolidinones as antiviral agents)

RN 214336-92-2 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aR,6R,6aS)-hexahydro-6-methyl-5-oxo-4-(2-thiazolyl)pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

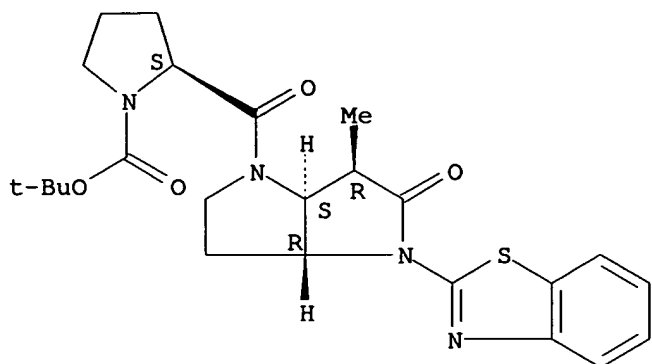


RN 214336-94-4 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aR,6R,6aS)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

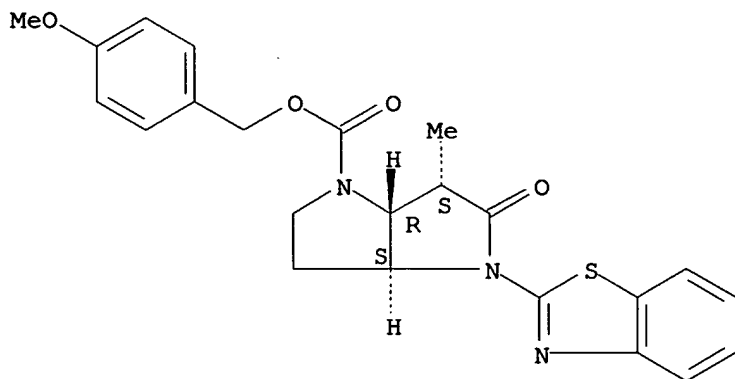
10/810,999



RN 214337-13-0 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-carboxylic acid, 4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxo-, (4-methoxyphenyl)methyl ester, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 214337-16-3 CAPLUS

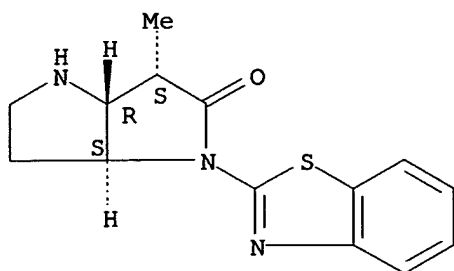
CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, 1-(2-benzothiazolyl)hexahydro-3-methyl-, (3S,3aR,6aS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 214337-15-2

CMF C14 H15 N3 O S

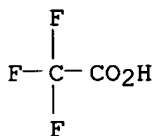
Absolute stereochemistry.



CM 2

CRN 76-05-1

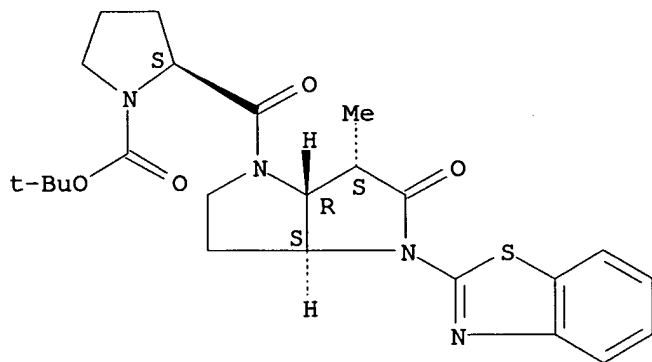
CMF C2 H F3 O2



RN 214337-18-5 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

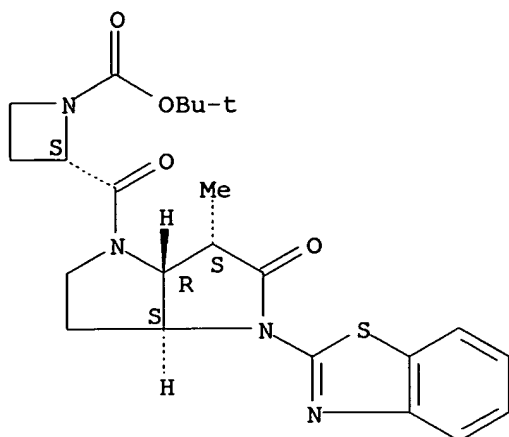
Absolute stereochemistry.



RN 214337-26-5 CAPLUS

CN 1-Azetidinecarboxylic acid, 2-[[(3aS,6S,6aR)-4-(2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

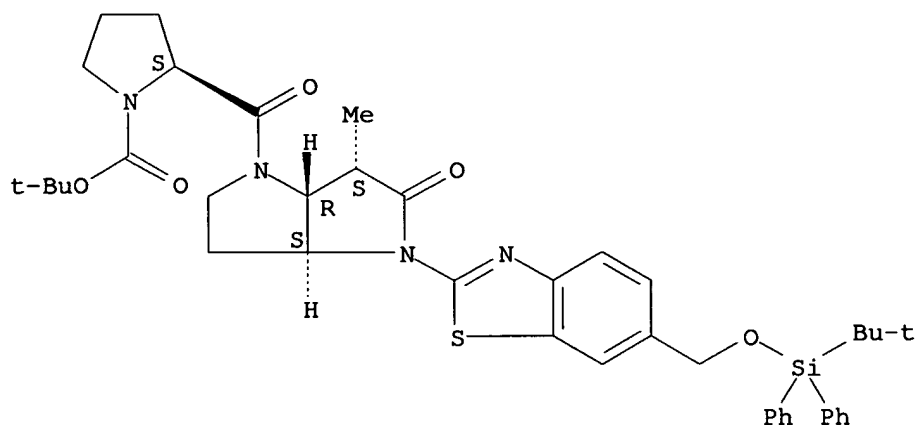
Absolute stereochemistry.



RN 214337-31-2 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-4-[6-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-benzothiazolyl]hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

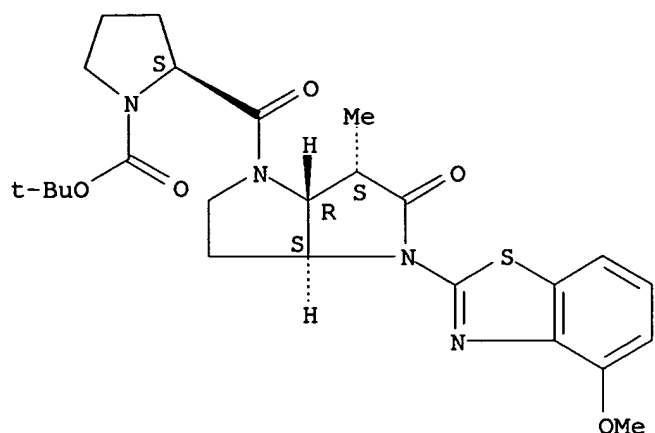
Absolute stereochemistry.



RN 214337-32-3 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-hexahydro-4-(4-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

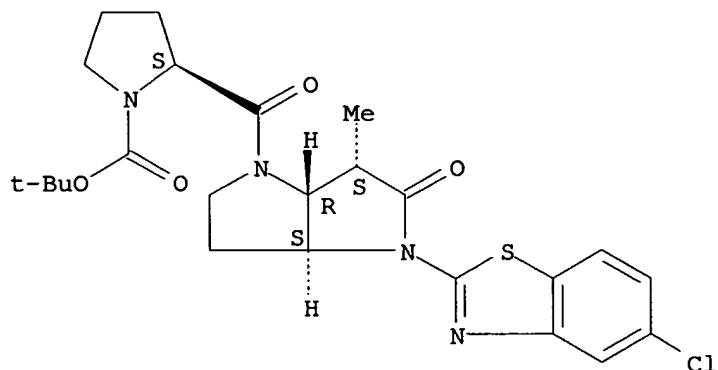
Absolute stereochemistry.



RN 214337-33-4 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-4-(5-chloro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

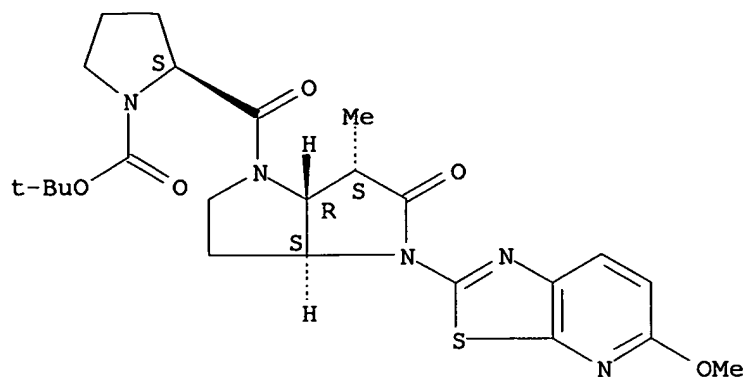
Absolute stereochemistry.



RN 214337-37-8 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-hexahydro-4-(5-methoxythiazolo[5,4-b]pyridin-2-yl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

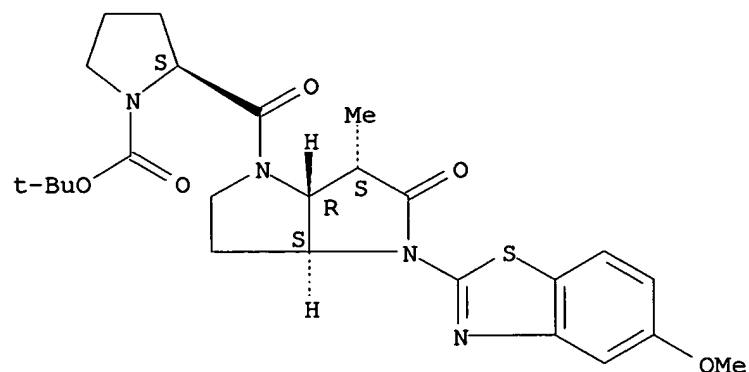
Absolute stereochemistry.



RN 214337-41-4 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-hexahydro-4-(5-methoxy-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

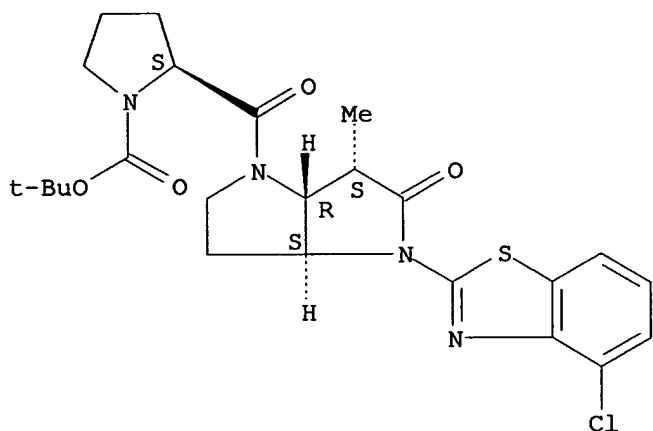
Absolute stereochemistry.



RN 214337-43-6 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-4-(4-chloro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

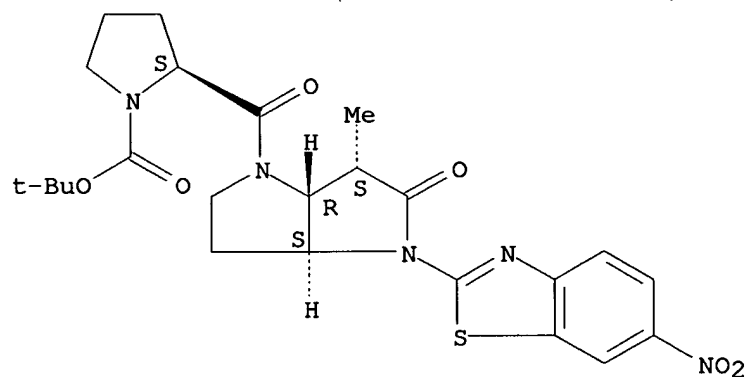
Absolute stereochemistry.



RN 214337-45-8 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-hexahydro-6-methyl-4-(6-nitro-2-benzothiazolyl)-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)-(9CI) (CA INDEX NAME)

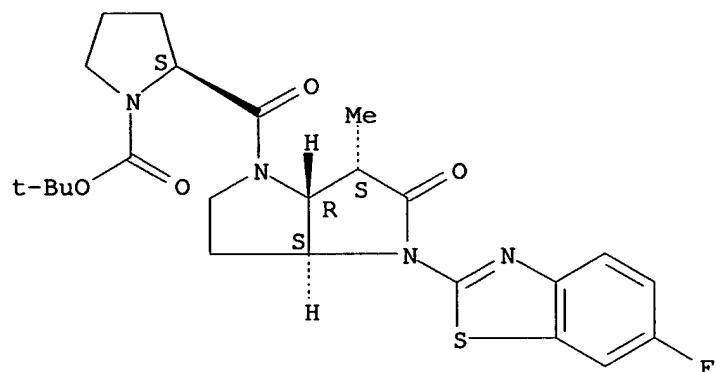
Absolute stereochemistry.



RN 214337-47-0 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[(3aS,6S,6aR)-4-(6-fluoro-2-benzothiazolyl)hexahydro-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)-(9CI) (CA INDEX NAME)

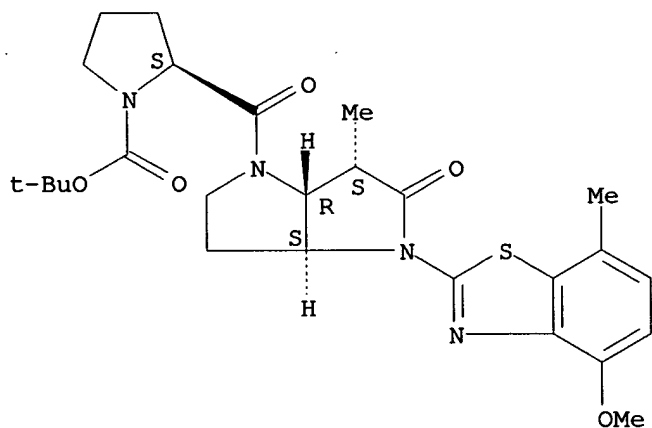
Absolute stereochemistry.



RN 214337-50-5 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-hexahydro-4-(4-methoxy-7-methyl-2-benzothiazolyl)-6-methyl-5-oxopyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

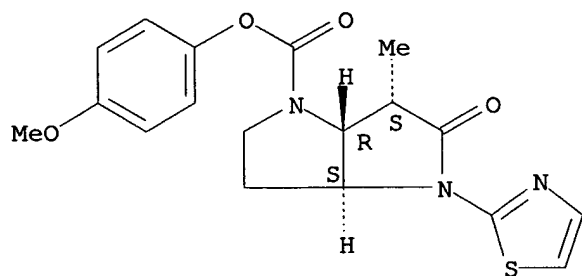
Absolute stereochemistry.



RN 214337-52-7 CAPLUS

CN Pyrrolo[3,2-b]pyrrole-1(2H)-carboxylic acid, hexahydro-6-methyl-5-oxo-4-(2-thiazolyl)-, 4-methoxyphenyl ester, (3aS,6S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



10/810,999

RN 214337-54-9 CAPLUS

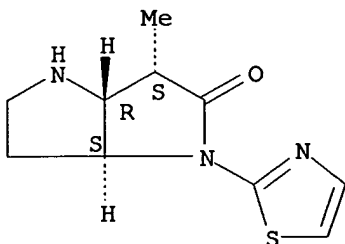
CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, hexahydro-3-methyl-1-(2-thiazolyl)-, (3S,3aR,6aS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 214337-53-8

CMF C10 H13 N3 O S

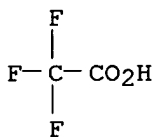
Relative stereochemistry.



CM 2

CRN 76-05-1

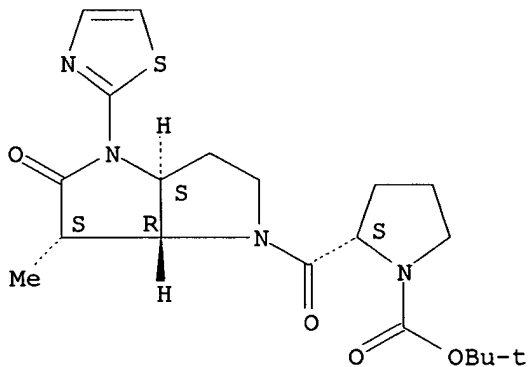
CMF C2 H F3 O2



RN 214337-55-0 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3aS,6S,6aR)-hexahydro-6-methyl-5-oxo-4-(2-thiazolyl)pyrrolo[3,2-b]pyrrol-1(2H)-yl]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



10/810,999

RN 214337-57-2 CAPLUS

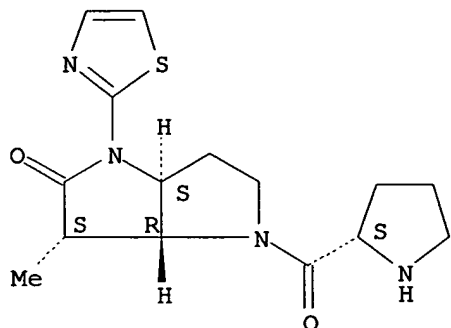
CN Pyrrolo[3,2-b]pyrrol-2(1H)-one, hexahydro-3-methyl-4-[(2S)-2-pyrrolidinylcarbonyl]-1-(2-thiazolyl)-, (3S,3aR,6aS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 214337-56-1

CMF C15 H20 N4 O2 S

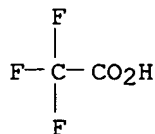
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~110~~ ANSWER 18 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:116497 CAPLUS

DOCUMENT NUMBER: 126:117990

TITLE: Preparation of quinolizinone- and pyridopyrimidinonecarboxylates as antibacterials

INVENTOR(S): Chu, Daniel T.; Li, Qun; Cooper, Curt S.; Fung, Anthony K. L.; Lee, Cheuk M.; Plattner, Jacob J.; Ma, Zhenkun; Wang, Wei-Bo

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 412 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

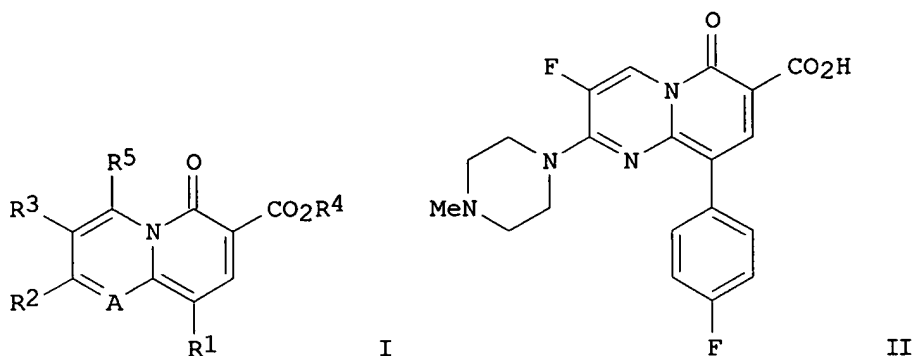
FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9639407	A1	19961212	WO 1996-US8991	19960605
W: AU, CA, IL, JP, KP, MX				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2222322	AA	19961212	CA 1996-2222322	19960605
AU 9661530	A1	19961224	AU 1996-61530	19960605
EP 871628	A1	19981021	EP 1996-919103	19960605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 11510478	T2	19990914	JP 1996-501420	19960605
PRIORITY APPLN. INFO.:			US 1995-469159	A 19950606
			US 1996-638112	A 19960529
			WO 1996-US8991	W 19960605

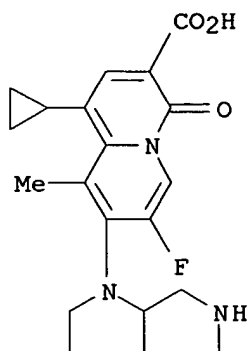
OTHER SOURCE(S): MARPAT 126:117990

GI



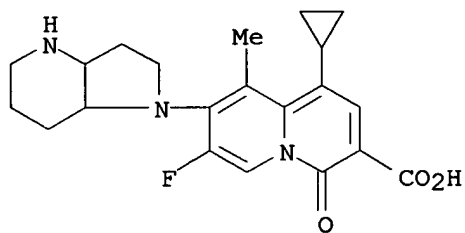
AB Title compds. [I; A = N or CR₆; R₁ = halo, (cyclo)alkyl, alkoxy, (un)substituted Ph, etc.; R₂ = halo, (cyclo)alkyl, alkoxy, N-containing heterocyclyl, etc.; R₃ = H, halo, alkoxy; R₄ = H, alkyl, cation, etc.; R₅, R₆ = H, halo, alkyl, alkoxy, etc.] were prepared Thus, 4-FC₆H₄CH₂C(:NH)NH₂ was cyclocondensed with NaOCH:CFCO₂Et (preparation given) and the chlorinated product aminated by 1-methylpiperazine to give 5-fluoro-2-(4-fluorobenzyl)-4-(4-methylpiperazino)pyrimidine which was condensed with EtOCH:C(CO₂Et)₂ and the product cyclized to give, in 2

addnl. steps, title compound II. Data for biol. activity of I were given.
 IT 169748-60-1P 186196-77-0P 186197-36-4P
 186198-11-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of quinolizine- and pyridopyrimidinonecarboxylates as antibacterials)
 RN 169748-60-1 CAPLUS
 CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)-9-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

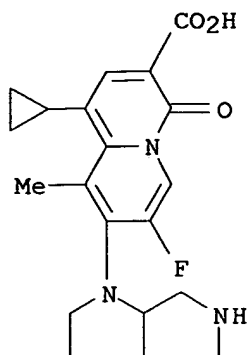
RN 186196-77-0 CAPLUS
 CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-1H-pyrrolo[3,2-b]pyridin-1-yl)-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

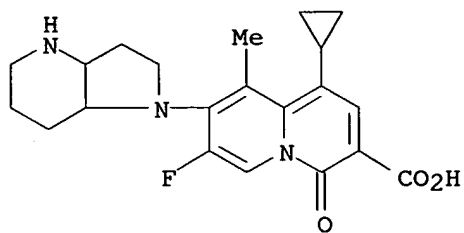
RN 186197-36-4 CAPLUS
 CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)-9-methyl-4-oxo- (9CI) (CA INDEX NAME)

10/810,999



RN 186198-11-8 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-1H-pyrrolo[3,2-b]pyridin-1-yl)-4-oxo- (9CI) (CA INDEX NAME)



~~DOI~~ ANSWER 19 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:422678 CAPLUS

DOCUMENT NUMBER: 125:221511

TITLE: Synthesis and Structure-Activity Relationships of 2-Pyridones: A Novel Series of Potent DNA Gyrase Inhibitors as Antibacterial Agents

AUTHOR(S): Li, Qun; Chu, Daniel T. W.; Claiborne, Akiyo; Cooper, Curt S.; Lee, Cheuk M.; Raye, Kathleen; Berst, Kristine B.; Donner, Pamela; Wang, Weibo; et al.

CORPORATE SOURCE: Abbott Laboratories, Abbott Park, IL, 60064-3500, USA
SOURCE: Journal of Medicinal Chemistry (1996), 39(16), 3070-3088

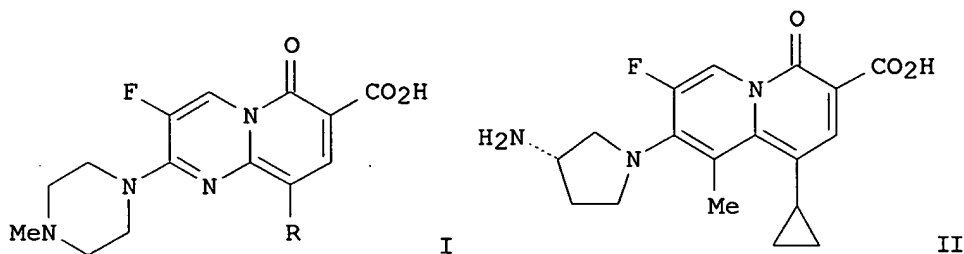
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Two novel series of 2-pyridones, e.g. I (R = 2,4-F₂C₆H₃), II, were synthesized by transposition of the nitrogen of 4-quinolones to the bridgehead position. This subtle interchange of the nitrogen atom with a carbon atom yielded two novel heterocyclic nuclei, pyrido[1,2-a]pyrimidine and quinolizine, which had not previously been evaluated as antibacterial agents and were found to be potent inhibitors of DNA gyrase. Quinolizines with a Me group at the 9-position such as II (ABT-719) demonstrate exceptional broad spectrum antibacterial activity. Most notably, they are active against resistant bacteria such as methicillin-resistant *Staphylococcus aureus*, vancomycin-resistant strains of enterococci, and ciprofloxacin-resistant organisms. In addition, 2-pyridones also possess favorable physiochem. and pharmacokinetic properties. These 2-pyridones were synthesized from the com. available starting materials by 10-17 linear transformations. The structure of an adduct yielded by this sequence, ABT-719, was determined by X-ray crystallog. anal.

IT 180975-97-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

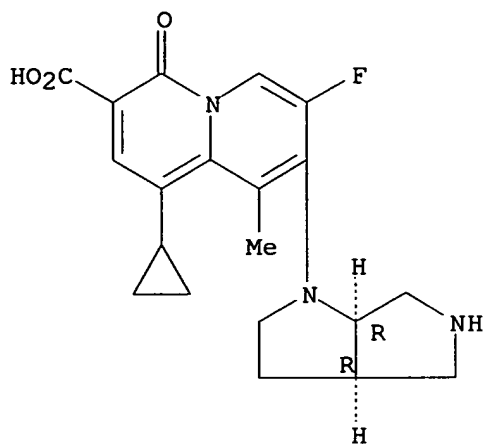
(preparation and bactericidal activity of 2-pyridones)

RN 180975-97-7 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)-9-methyl-4-oxo-, dihydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

10/810,999



● 2 HCl

~~10~~ ANSWER 20 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:892832 CAPLUS

DOCUMENT NUMBER: 123:313930

TITLE: Preparation of quinolizinonecarboxylates and analogs as antibacterials

INVENTOR(S): Chu, Daniel T.; Li, Qun; Cooper, Curt S.; Fung, Anthony K. L.; Lee, Cheuk M.; Plattner, Jacob J.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 255 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

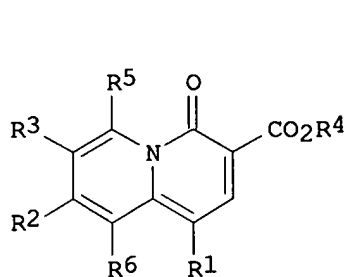
FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

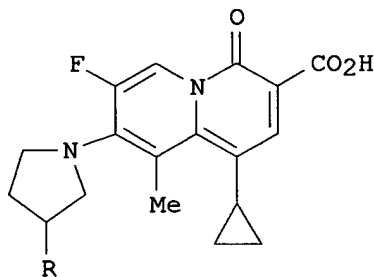
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9510519	A1	19950420	WO 1994-US11166	19940930
W: AU, BR, CA, CN, JP, KR				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2173459	AA	19950420	CA 1994-2173459	19940930
AU 9479258	A1	19950504	AU 1994-79258	19940930
AU 689809	B2	19980409		
EP 723545	A1	19960731	EP 1994-929998	19940930
EP 723545	B1	20020508		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CN 1137273	A	19961204	CN 1994-194479	19940930
CN 1053188	B	20000607		
JP 09503783	T2	19970415	JP 1994-511876	19940930
BR 9407806	A	19970819	BR 1994-7806	19940930
AT 217309	E	20020515	AT 1994-929998	19940930
PRIORITY APPLN. INFO.:			US 1993-137236	A 19931014
			WO 1994-US11166	W 19940930

OTHER SOURCE(S): MARPAT 123:313930

GI



I



II

AB Title compds. [I; R1 = halo, (cyclo) alkyl, Ph, heterocyclyl, etc.; R2 = halo, (cyclo)alk(en)yl, Ph, heterocyclyl, etc.; R3 = H, halo, alkoxy; R4 = H, alkyl, cation, ester residue; R5 = H, halo, OH, alkyl, etc.; R6 = alkyl] were prepared. Thus, 3-chlorotetrafluoropyridine was converted in a multistep synthesis to 2-(4-chloro-5-fluoro-3-methyl-2-pyridyl)cyclopropaneacetaldehyde which was condensed with CH2(CO2Et)2 and the product cyclized to give, after amination, title compound (R)-II.HCl [R = (S)-CH(NH2)Et] which had MIC of 0.05 and 12.5 µg/mL against

10/810,999

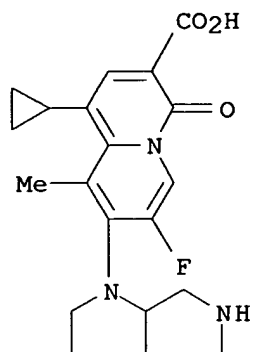
Staphylococcus aureus 1775 and Candida albicans CCH 442, resp.

IT **169748-60-1P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinolizinonecarboxylates and analogs as antibacterials)

RN 169748-60-1 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-(hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)-9-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

110 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:511584 CAPLUS

DOCUMENT NUMBER: 117:111584

TITLE: Preparation of 7-[2,7-diazabicyclo[3.3.0]-3-quinolone- and -naphthyridonocarboxylates as bactericides

INVENTOR(S): Petersen, Uwe; Schenke, Thomas; Schriewer, Michael; Grohe, Klaus; Krebs, Andreas; Haller, Ingo; Metzger, Karl Georg; Bremm, Klaus Dieter; Endermann, Rainer; Zeiler, Hans Joachim

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Ger. Offen., 43 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

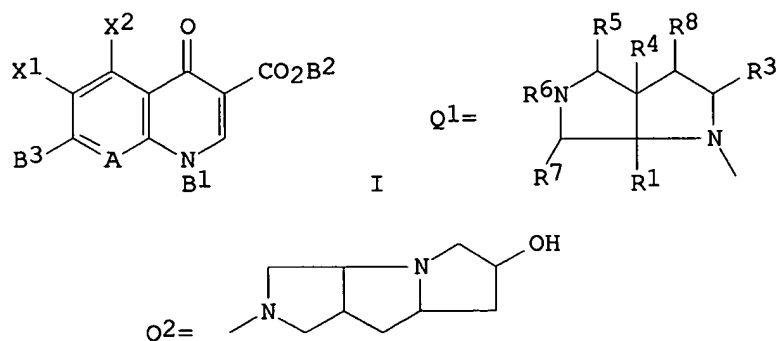
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4032560	A1	19920416	DE 1990-4032560	19901013
EP 481274	A1	19920422	EP 1991-116651	19910930
EP 481274	B1	19961023		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 144514	E	19961115	AT 1991-116651	19910930
ES 2093666	T3	19970101	ES 1991-116651	19910930
US 5202337	A	19930413	US 1991-771700	19911003
JP 04282384	A2	19921007	JP 1991-287162	19911007
US 5284855	A	19940208	US 1992-974446	19921112
PRIORITY APPLN. INFO.:			DE 1990-4032560	A 19901013
			US 1991-771700	A3 19911003

OTHER SOURCE(S): MARPAT 117:111584

GI



AB Title compds. [I; X1 = halo; X2 = H, NH₂, (di)alkylamino, OH, alkoxy, SH, alkylthio, arylthio, halo, Me; A = N, CR₉; B1 = (cyclo)alkyl, alkenyl, OMe, NH₂, etc.; B2 = H, alkyl, etc.; B3 = diazabicyclooctyl group, e.g., Q1 and analogs; R1, R3-R5, R7, R8 = H, (halo)methyl, CO₂H, alkoxy carbonyl, etc. R4, R8 may addnl. = halo, NH₂, OH, OMe; R6 = H, alkyl, PhCH₂, aryl, alkanoyl, Bz, alkoxy carbonyl; R9 = H, halo, Me, cyano, OH, etc.; R9B1 = OCH₂CHMe, SCH₂CHMe, CH₂CH₂CHMe] were prepared Thus, CH₂:CHCH₂N(CO₂Et)CH₂CHO

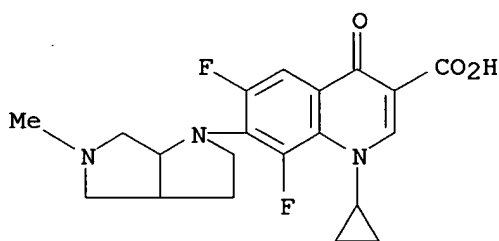
was cyclocondensed with trans-4-hydroxyproline and the product saponified and decarboxylated to give R2H (R2 = diazatricycloundecano group Q2) which was condensed with I (A = CF, B1 = cyclopropyl, B2 = X2 = H, X1 = F, B3 = F) (II) to give II (B3 = Q2). II (B3 = Q1, X1 = F, X2 = B2 = H, B1 = cyclopropyl, R1 = R3 = R5 = R6 = R7 = R8 = H, R4 = Cl) had MIC of 0.03 and 4 mg/L against Escherichia coli Neumann and Staphylococcus aureus ICB 25701, resp.

IT 142345-37-7P 142345-38-8P 142345-39-9P
 142345-40-2P 142345-41-3P 142345-42-4P
 142345-43-5P 142345-44-6P 142345-45-7P
 142345-46-8P 142345-47-9P 142345-48-0P
 142345-49-1P 142345-50-4P 142345-51-5P
 142345-52-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as bactericide)

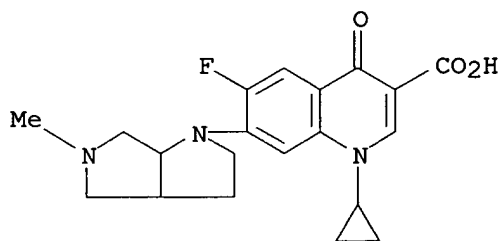
RN 142345-37-7 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-7-(hexahydro-5-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



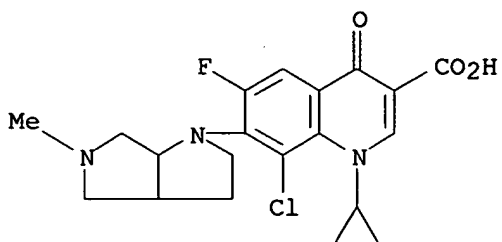
RN 142345-38-8 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6-fluoro-7-(hexahydro-5-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



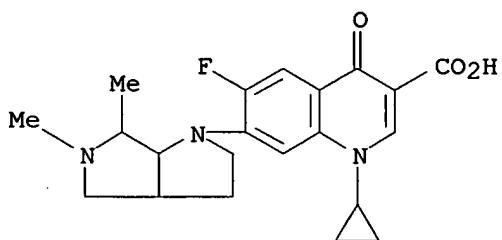
RN 142345-39-9 CAPLUS

CN 3-Quinolinecarboxylic acid, 8-chloro-1-cyclopropyl-6-fluoro-7-(hexahydro-5-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



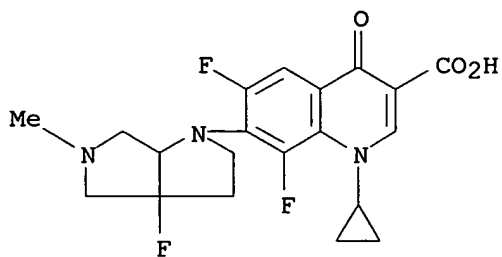
RN 142345-40-2 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6-fluoro-7-(hexahydro-5,6-dimethylpyrrolo[3,4-b]pyrrol-1(2H)-yl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



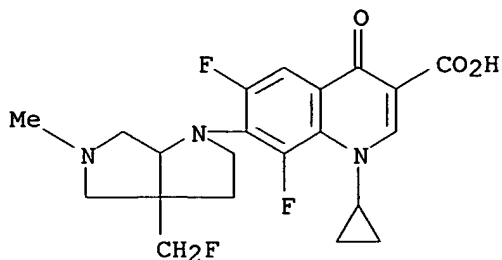
RN 142345-41-3 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-7-(3a-fluorohexahydro-5-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl)-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



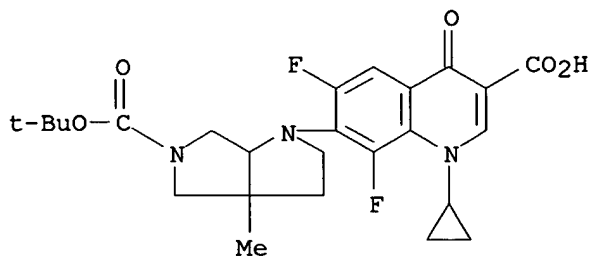
RN 142345-42-4 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-7-[3a-(fluoromethyl)hexahydro-5-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



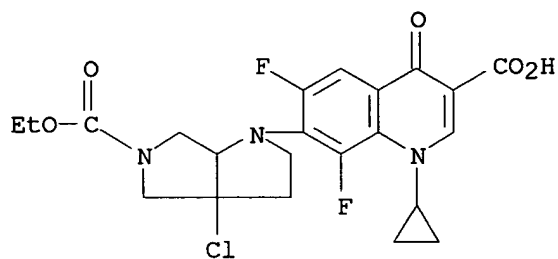
RN 142345-43-5 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-7-[5-[(1,1-dimethylethoxy)carbonyl]hexahydro-3a-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl]-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



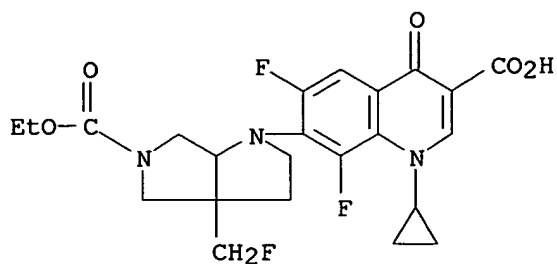
RN 142345-44-6 CAPLUS

CN 3-Quinolinecarboxylic acid, 7-[3a-chloro-5-(ethoxycarbonyl)hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



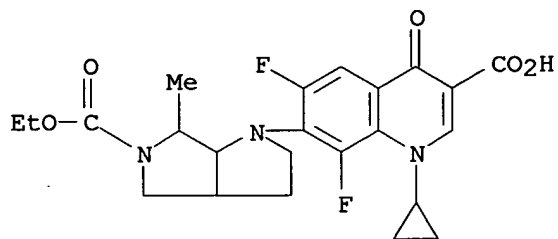
RN 142345-45-7 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-7-[5-(ethoxycarbonyl)-3a-(fluoromethyl)hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



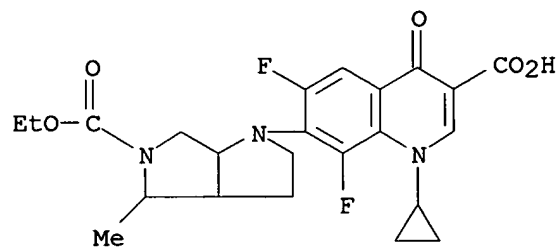
RN 142345-46-8 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-7-[5-(ethoxycarbonyl)hexahydro-6-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl]-6,8-difluoro-1,4-dihydro-4-oxo- (9CI)
(CA INDEX NAME)



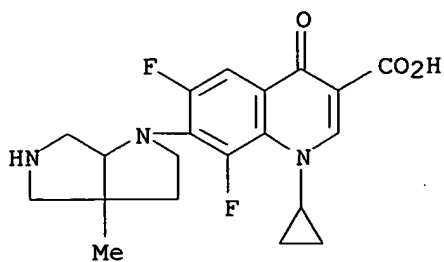
RN 142345-47-9 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-7-[5-(ethoxycarbonyl)hexahydro-4-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl]-6,8-difluoro-1,4-dihydro-4-oxo- (9CI)
(CA INDEX NAME)



RN 142345-48-0 CAPLUS

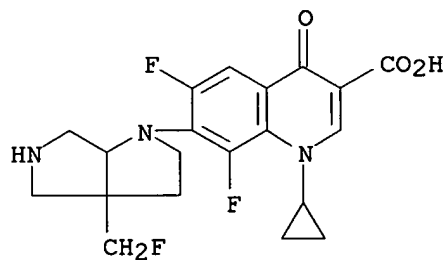
CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-7-(hexahydro-3a-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl)-1,4-dihydro-4-oxo-, hydrochloride
(9CI) (CA INDEX NAME)



●x HCl

RN 142345-49-1 CAPLUS

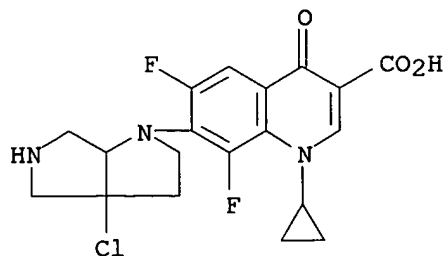
CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-7-[3a-(fluoromethyl)hexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl]-1,4-dihydro-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

RN 142345-50-4 CAPLUS

CN 3-Quinolinecarboxylic acid, 7-(3a-chlorohexahydropyrrolo[3,4-b]pyrrol-1(2H)-yl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)

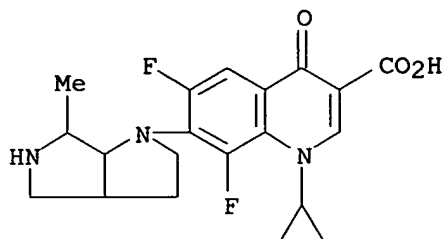


●x HCl

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RN 142345-51-5 CAPLUS

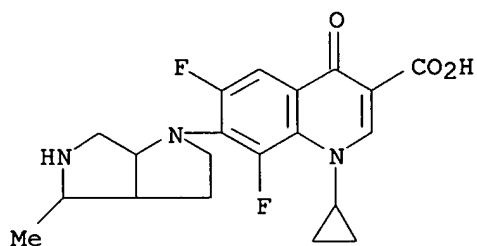
CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-7-(hexahydro-6-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl)-1,4-dihydro-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

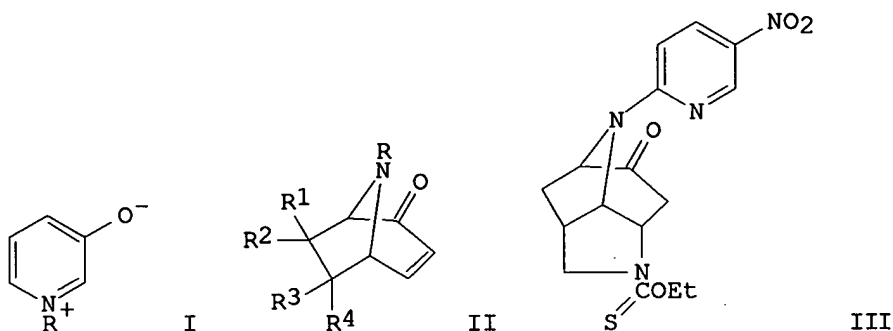
RN 142345-52-6 CAPLUS

CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6,8-difluoro-7-(hexahydro-4-methylpyrrolo[3,4-b]pyrrol-1(2H)-yl)-1,4-dihydro-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

~~EN~~ ANSWER 22 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1984:571135 CAPLUS
 DOCUMENT NUMBER: 101:171135
 TITLE: 1,3-Dipolar cycloaddition reactions of some
 six-membered aromatic betaines
 AUTHOR(S): Turker, Lemi; Guner, Fatih
 CORPORATE SOURCE: USA
 SOURCE: Muslim Scientist (1983), 12(3), 12-21
 CODEN: MUSCDX; ISSN: 0148-0995
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Oxidopyridinium betaines I (R = 5-nitro-2-pyridyl; 4,6-dimethyl-2-pyrimidinyl) underwent cycloaddn. with dipolarophiles. For example, treating I (same R) with HOCH₂CH₂C.tplbond.CH gave azabicyclooctadienes II (R₁R₃ = bond; R₂ = H, R₄ = CHMeOH; R₂ = CHMeOH, R₄ = H). I (R = 5-nitro-2-pyridyl) reacted with H₂C:CHR₅ (R₅ = succinimido) to form endo and exo adducts II (R₁-R₃ = H, R₄ = R₅; R₁ = R₅, R₂-R₄ = H), and with H₂C:CHCH₂NCS to give II (R₁-R₃ = H, R₄ = CH₂NCS). The last underwent cyclization with ethanolic HCl to give diazatricyclodecanone III.

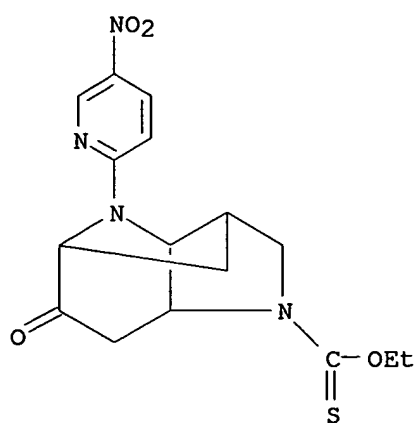
IT **92486-24-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

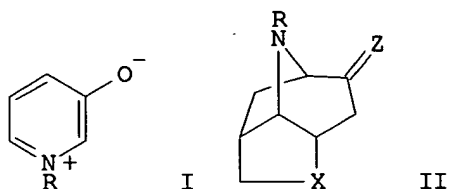
RN 92486-24-3 CAPLUS

CN 3,5-Methano-1H-pyrrolo[3,2-b]pyridine-1-carbothioic acid,
 octahydro-4-(5-nitro-2-pyridinyl)-6-oxo-, O-ethyl ester (9CI) (CA INDEX
 NAME)

10/810,999

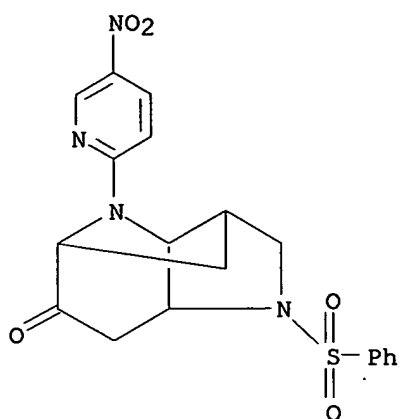


~~110~~ ANSWER 23 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1979:611292 CAPLUS
 DOCUMENT NUMBER: 91:211292
 TITLE: 1,3-Dipolar character of six-membered aromatic rings.
 Part 43. Cycloadditions leading to tricyclic adducts
 AUTHOR(S): Katritzky, Alan R.; Dennis, Nicholas; Sabongi, Gebran
 J.; Turker, Lemi
 CORPORATE SOURCE: Sch. Chem. Sci., Univ. East Anglia, Norwich, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1979), (6), 1525-35
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 91:211292
 GI



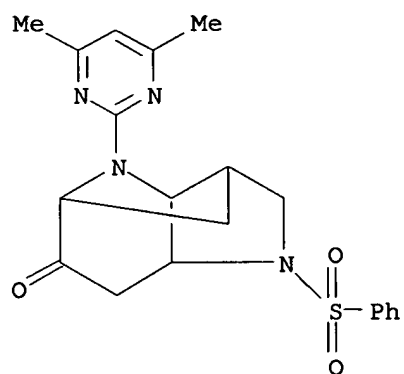
AB CH₂:CHCH₂OH reacted with the pyridiniums I (R = 5-nitro-2-pyridyl, 4,6-dimethylpyrimidin-2-yl, 4,6-dimethoxy-1,3,5-triazin-2-yl), generated in situ either from their corresponding salts or dimers, to give tricyclic products II (X = Z = O, R as before) in which the OH group has added to the α,β -unsatd. ketone. Analogous products were obtained from PhSO₂NHCH₂CH:CH₂, CH₂:CHCO₂H, and 2-vinylpyridine. Thus, I (R = 5-nitro-2-pyridyl) with PhSO₂NHCH₂CH:CH₂ gave 22% II (X = NSO₂Ph, Z, R as before). II (R = 4,6-dimethylpyrimidin-2-yl, Z = X = O) reacted with PhNHNH₂ to give 96% II (Z = NNHPh, X, R as before). Further transformations of the primary adducts are described.
 IT **71902-71-1P 71902-73-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 71902-71-1 CAPLUS
 CN 3,5-Methano-6H-pyrrolo[3,2-b]pyridin-6-one, octahydro-4-(5-nitro-2-pyridinyl)-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

10/810,999



RN 71902-73-3 CAPLUS

CN 3,5-Methano-6H-pyrrolo[3,2-b]pyridin-6-one, 4-(4,6-dimethyl-2-pyrimidinyl)octahydro-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



110 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:588296 CAPLUS

DOCUMENT NUMBER: 83:188296

TITLE: Synthesis and pharmacological activity of
4-amino-3-nitrocoumarins

AUTHOR(S): Savel'ev, V. L.; Pryanishnikova, N. T.; Artamonova, O.
S.; Fedina, I. V.; Zagorevskii, V. A.

CORPORATE SOURCE: Inst. Farmakol., Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1975), 9(6), 10-12
CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 83:188296

GI For diagram(s), see printed CA Issue.

AB Of 17 4-amino-3-nitrocoumarins (I) prepared and tested for pharmacol.
activity in mice and rabbits, 15 had neurotropic activity, generally
inhibiting spontaneous locomotor activity, decreasing hyperactivity
induced by phenamine, and prolonging thiopental sleep. The compound containing
a primary amino group (I, R = NH₂ [38464-21-0]) decreased spontaneous
activity 6-10-fold, prolonged thiopental sleep 30%, and somewhat enhanced
phenamine hyperactivity. The most active of the derivs. containing a
secondary amino group (I, R = NHC₆H₁₁ [56962-68-6]) inhibited phenamine
hyperactivity 2-5-fold and prolonged thiopental sleep 2-fold. The most
active of the compds. containing a tertiary amino group was I, R = NEt₂
[50527-31-6]. The compound I, R = 1,4-diazabicyclo[4,3,0]nonan-1-yl [**56990-99-9**]
decreased motor activity 3-4-fold, prolonged
thiopental sleep 1.5-1.7-fold, and decreased phenamine hyperactivity.
None of the compds. had analgetic, anesthetic, or muscle relaxant
properties.

IT **56990-99-9P**

RL: BAC (Biological activity or effector, except adverse); BPR (Biological
process); BSU (Biological study, unclassified); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); PROC (Process); USES (Uses)
(preparation and pharmacol. of)

RN 56990-99-9 CAPLUS

CN 2H-1-Benzopyran-2-one, 3-nitro-4-(octahydro-1H-pyrrolo[3,2-b]pyridin-1-yl)-
(9CI) (CA INDEX NAME)

